Physics of Elasticity and Defects

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Also by Adrian P. Sutton:

Electronic structure of materials, Oxford University Press: Oxford (1993), 260 pages + xv. Reprinted 1994, 1996. Published in German translation as *Elektronische Struktur in Materialen*, by VCH: Weinheim, in 1996.

Interfaces in crystalline materials, with R W Balluffi, Oxford University Press (1995), 819 pages + xxxi. Reprinted 1996. Reissued in 2006 in the series *Classic Texts in the Physical Sciences*, Oxford University Press: Oxford. Published in Chinese in 2015 by the Higher Education Press Limited Company: Beijing.

Contents

Preface

The first six chapters of this book are based on a postgraduate course I have given in the Centre for Doctoral Training (CDT) on Theory and Simulation of Materials at Imperial College London since 2009. The last four chapters cover material that I would have included in the course had there been more time available. The CDT was created in 2009 to attract first class physicists and engineers with a taste for theory into materials science, to expose them to research areas of a theoretical nature they would not normally encounter in their own departments. Working with multidisciplinary teams of academic staff, our CDT students have opened up new areas of materials physics to theory and simulation.

The course is about defects and their elastic interactions in crystalline materials. Some justification is needed for another book in an area which already benefits from some excellent texts, some of which are listed in the Bibliography. By discussing the connections to treatments of defects at the atomic scale I have tried to make the text more appealing to physicists. At the same time this approach is quite novel for engineers. Even the treatments of strain and stress in the first two chapters contain sections that will be new to students of engineering. Having given this course to physics graduates from the UK and continental Europe I know that most, in many cases all, the material covered in this course was new to them.

Until the late 1960s, in some of the strongest departments of physics around the world, 'metal physics' was focused on the physics of defects and their interactions. But today such metal physics has become unfashionable and it has vanished almost completely from physics departments. The study of metals and alloys by physicists has metamorphosed into functional properties such as superconductivity, plasmonics and magnetism. Undergraduate courses of physics rarely include anything on defects in crystals, other than dopants in semiconductors, so physics students could be forgiven for thinking the world is made of perfect single crystals. But the industrial need for an understanding of defect-related mechanisms of mechanical failures has become greater. Major manufacturing companies have recognised they cannot make reliable assessments of the life-times of components critical for safety unless they understand at a more fundamental level how and why they fail. On the other hand, engineering departments do not have a tradition of thinking about materials down to the atomic scale. For example, hydrogen embrittlement is a problem that

cuts across swathes of current and proposed technologies, but it has fallen between physics and engineering, and very little progress has been made into the fundamental mechanisms. I have written this book because the physics of defects will remain important as long as we use metals and alloys to make things like jet engines, cars, bridges, skyscapers and nuclear power stations, and because it treats the subject in a way that I hope will appeal more to students with backgrounds in physics and engineering.

This book is *not* self-contained and there is a bibliography at the end which should be consulted. In chapter 6 it is essential to read Hull and Bacon if you have no previous knowledge of dislocations. I have also included references to research papers in the footnotes with links to the urls where they can be found.

The theory of elasticity has a long history going back to Euler in the 18th century. Its evolution through the 19th and 20th centuries involved some of the most familiar names in the development of mathematical science. In footnotes I have included brief information about these people. It will be seen that many of them were Fellows of the Royal Society (FRS), with one President of the Royal Society (PRS) and one Foreign Member of the Royal Society (ForMemRS). The Royal Society is the National Academy of Sciences in the UK, and it is the oldest of all the national academies. The subject is still evolving and the final chapter introduces four areas where fundamental questions remain unanswered, and where further research is needed.

I am very grateful to my colleagues in the Department of Physics at Imperial College London who in 2004 took the bold decision to hire a materials scientist, and thus allow a Trojan Horse into their midst to recruit some of their best students into materials physics. I have been encouraged and supported in all my work at Imperial by colleagues across the nine departments involved in our CDT. The period since I founded the CDT in 2009 has been the most creative of my research and teaching career. None of this would have been possible without the wonderful students we have managed to attract to the CDT, and it is to them that I dedicate this book.

1. Strain

1.1 The continuum approximation

Condensed matter is lumpy. It comprises very dense atomic nuclei packed together a few Ångstroms apart, with electrons in much less dense clouds around them. The continuum approximation smears out this lumpiness into a uniform, structureless jelly with the same density as a macroscopic lump of the matter it approximates. In addition to its density the continuum is given elastic properties, which characterise how easy it is to deform it in a reversible manner. The elastic properties of the continuum are equated to those of the material it approximates.

What physics do we leave out by approximating the discrete atomic structure of a material with a continuum model? Whenever the discrete atomic structure of the material becomes essential to the physics we can expect the continuum model to be a poor approximation. For example, when we consider structural defects inside the material we can expect the continuum model to become increasingly unreliable as we get closer to the centre of the defect because there the discrete atomic structure of the defect can no longer be ignored. But once we get beyond a few nanometres, in many cases just one nanometre, from the centre of a defect the continuum approximation becomes an accurate description of the distortion the defect generates.

Whereas the smallest separation of atoms in a material provides a natural length-scale there is no natural length-scale associated with the continuum. This has significant consequences for dynamical properties, such as the propagation of atomic vibrations. There are just three waves that can propagate in the continuum with speeds that vary in general with the direction of propagation. In contrast to phonons in a crystal the elastic waves are dispersionless, i.e. their speed of propagation does not depend on their wavelength. The dispersion of phonons in a crystal is a direct consequence of its discrete atomic structure. Waves in the crystal and in its continuum representation coincide only in the limit of long wavelengths compared with the spacing of atoms, where the discreteness of the atomic structure no longer plays a significant role in wave propagation.

1.2 What is deformation?

When a body changes shape or volume in response to external or internal forces it is *deformed*. In contrast to a rigid rotation or translation, deformation alters distances between points within the body. Materials may undergo changes of volume and shape in response to changes of temperature, applied electric and magnetic fields and other fields including gravitational. In this book we will be concerned principally with deformation created by mechanical forces applied to bodies and by defects within them. The focus of this chapter is the mathematical description of deformation and strain.

The simplest deformation is a homogeneous expansion or contraction where the distance between any two points changes by an amount proportional to their separation in the undeformed state. The word 'homogeneous' here means 'the same everywhere'. When a body is deformed inhomogeneously the deformation depends on position in the undeformed state. The deformation is then a *field*.

Let $\mathbf{X}$ be the position vector of a point in the body before any deformation occurs. Let $\mathbf{X}+\mathrm{d}\mathbf{X}$ be the position vector of a point in the undeformed body infinitesimally close to $\mathbf{X}$. These two points are separated by $|\mathrm{d}\mathbf{X}| = \sqrt{\mathrm{d}X_i\,\mathrm{d}X_i}$, where X_i is Cartesian component i of $\mathbf{X}$, and summation is implied here and throughout this book whenever subscripts are repeated. Thus, $\mathrm{d}X_i\,\mathrm{d}X_i$ is shorthand for $\mathrm{d}X_1^2+\mathrm{d}X_2^2+\mathrm{d}X_3^2$.

Suppose $\mathbf{X}$ and $\mathbf{X}+\mathrm{d}\mathbf{X}$ become $\mathbf{x}$ and $\mathbf{x}+\mathrm{d}\mathbf{x}$ in the deformed state. In general $\mathbf{x}$ is a function of $\mathbf{X}$. The chain rule enables us to write down the components of $\mathrm{d}\mathbf{x}$ in terms of the components of $\mathrm{d}\mathbf{X}$:

$$\mathrm{d}x_i = \frac{\partial x_i}{\partial X_j}\mathrm{d}X_j \tag{1.1}$$

The 3×3 matrix $F_{ij} = \partial x_i/\partial X_j$ is called the *deformation tensor* . It follows that the change in the squared separation of the points is given by:

$$\mathrm{d}x_i\mathrm{d}x_i - \mathrm{d}X_j\mathrm{d}X_j = \left(\frac{\partial x_i}{\partial X_j}\frac{\partial x_i}{\partial X_k} - \delta_{jk}\right)\mathrm{d}X_j\mathrm{d}X_k, \tag{1.2}$$

where δ_{jk} is the Kronecker delta: $\delta_{jk}=1$ if $j=k$, and $\delta_{jk}=0$ if $j\neq k$.

Exercise 1.1 (i) Prove that the deformation tensor F_{ij} satisfies the tensor transformation law under a rotation of the coordinate system. This is what defines F_{ij} as a tensor.
(ii) Show that in matrix notation eqn.(1.2) becomes:

$$(\mathrm{d}\mathbf{x}^T\cdot\mathrm{d}\mathbf{x}) - (\mathrm{d}\mathbf{X}^T\cdot\mathrm{d}\mathbf{X}) = \mathrm{d}\mathbf{X}^T\cdot\left(\mathbf{F}^T\mathbf{F}-\mathbf{I}\right)\cdot\mathrm{d}\mathbf{X}$$

where the T superscript denotes transpose, and $\mathbf{I}$ is the identity matrix.
(iii) Hence prove that if the deformation tensor is a rotation the change in the separation of points is zero. ∎

You may recognise $\mathbf{F}^T\mathbf{F}$ as the metric tensor $\mathbf{g}$ which measures the distance between two points in the deformed state. Consider first the distance between two points in the *undeformed* state. If $\mathbf{X}=\mathbf{X}(\lambda)$ is a parametric equation of a path in the undeformed state between two points A and B, where $\lambda=\lambda_A$ and $\lambda=\lambda_B$ respectively, then the distance between these points along the path in the undeformed state is given by

$$
\begin{aligned}
s &= \int_{\lambda=\lambda_A}^{\lambda=\lambda_B} \sqrt{\left(\frac{\mathrm{d}X_1}{\mathrm{d}\lambda}\right)^2 + \left(\frac{\mathrm{d}X_2}{\mathrm{d}\lambda}\right)^2 + \left(\frac{\mathrm{d}X_3}{\mathrm{d}\lambda}\right)^2}\,\mathrm{d}\lambda \\
&= \int_{\lambda=\lambda_A}^{\lambda=\lambda_B} \sqrt{\frac{\mathrm{d}X_i}{\mathrm{d}\lambda}\delta_{ij}\frac{\mathrm{d}X_j}{\mathrm{d}\lambda}}\,\mathrm{d}\lambda \\
&= \int_{\lambda\lambda_A}^{\lambda=\lambda_B} \sqrt{\frac{\mathrm{d}X_i}{\mathrm{d}\lambda}g_{ij}\frac{\mathrm{d}X_j}{\mathrm{d}\lambda}}\,\mathrm{d}\lambda
\end{aligned}
$$

and we see the metric tensor in the undeformed state is the identity matrix.

In the *deformed* state the path becomes $\mathbf{x} = \mathbf{x}(\mathbf{X}(\lambda))$ and points A and B are moved to new positions. The distance between points A and B along the deformed path is given by

$$
s = \int_{\lambda=\lambda_A}^{\lambda=\lambda_B} \sqrt{\mathrm{d}x_k(\lambda)\mathrm{d}x_k(\lambda)} = \int_{\lambda=\lambda_A}^{\lambda=\lambda_B} \sqrt{\frac{\mathrm{d}X_i}{\mathrm{d}\lambda}\frac{\partial x_k}{\partial X_i}\frac{\partial x_k}{\partial X_j}\frac{\mathrm{d}X_j}{\mathrm{d}\lambda}}\,\mathrm{d}\lambda, \tag{1.3}
$$

and the metric tensor is $g_{ij} = (\partial x_k/\partial X_i)(\partial x_k/\partial X_j)$, or $\mathbf{g} = \mathbf{F}^T\mathbf{F}$ in matrix notation. This is the point of departure for an analysis of deformation using the machinery of differential geometry, with similarities to some aspects of general relativity[1].

1.3 The displacement vector and the strain tensor

We may always express $\mathbf{x}(\mathbf{X})$ as $\mathbf{X} + \mathbf{u}(\mathbf{X})$, where $\mathbf{u}(\mathbf{X})$ is the displacement undergone by a point at $\mathbf{X}$ in the undeformed body when the body is deformed. The gradient of the displacement vector is related to the deformation tensor as follows:

$$
F_{ki} = \frac{\partial x_k}{\partial X_i} = \delta_{ki} + \frac{\partial u_k}{\partial X_i}. \tag{1.4}
$$

Exercise 1.2 Show that the squared separation of points that were at $\mathbf{X}$ and $\mathbf{X} + \mathrm{d}\mathbf{X}$ in the undeformed state becomes the following in the deformed state:

$$
(\mathrm{d}s)^2 = \left(\delta_{kj} + \frac{\partial u_k}{\partial X_j} + \frac{\partial u_j}{\partial X_k} + \frac{\partial u_i}{\partial X_k}\frac{\partial u_i}{\partial X_j}\right)\mathrm{d}X_k\mathrm{d}X_j \tag{1.5}
$$

■

Eqn.(1.5) is exact provided $|\mathrm{d}\mathbf{X}|$ is infinitesimal, and it leads to non-linear theories of elasticity. To obtain a linear approximation the assumption is made that the *gradients* of the displacement vector are small in comparison to unity. It is important to recognise that this assumption does not require the displacements themselves to be small. Taking the square root of both sides of eqn.(1.5), and dividing both sides by $|\mathrm{d}\mathbf{X}|$, we obtain:

[1] see *Geometrical Foundations of Continuum Mechanics*, Paul Steinmann, Springer-Verlag: Berlin (2015)

$$\begin{aligned}\frac{\mathrm{d}s}{|\mathrm{d}\mathbf{X}|} &= \sqrt{1+\hat{l}_k\left(\frac{\partial u_k}{\partial X_j}+\frac{\partial u_j}{\partial X_k}+\frac{\partial u_i}{\partial X_k}\frac{\partial u_i}{\partial X_j}\right)\hat{l}_j} \\ &\approx 1+\hat{l}_k e_{kj}\hat{l}_l, \end{aligned} \tag{1.6}$$

where the unit vector $\hat{\mathbf{l}}$ is parallel to $\mathrm{d}\mathbf{X}$ and e_{kj} is the *strain tensor*:

$$e_{kj} = \frac{1}{2}\left(\frac{\partial u_k}{\partial X_j}+\frac{\partial u_j}{\partial X_k}+\frac{\partial u_i}{\partial X_k}\frac{\partial u_i}{\partial X_j}\right) \tag{1.7}$$

Since the displacement gradients are assumed to be small the last term in eqn.(1.7) is neglected and thus we obtain the strain tensor used in linear elasticity, and in the rest of this book:

$$e_{kj} = \frac{1}{2}\left(\frac{\partial u_k}{\partial X_j}+\frac{\partial u_j}{\partial X_k}\right). \tag{1.8}$$

We see the strain tensor is symmetric. The displacement gradient may also contain an asymmetric part:

$$\frac{\partial u_k}{\partial X_j} = e_{kj}+\omega_{kj}$$

where $\omega_{kj} = \frac{1}{2}\left(\partial u_k/\partial X_j - \partial u_j/\partial X_k\right)$ is asymmetric because $\omega_{kj} = -\omega_{jk}$.

Exercise 1.3 Given the following general expression for the rotation matrix describing a rotation by θ about an axis $\hat{\boldsymbol{\rho}}$:

$$R_{ij} = \cos\theta\,\delta_{ij} + \hat{\rho}_i\hat{\rho}_j(1-\cos\theta) - \varepsilon_{ijk}\hat{\rho}_k\sin\theta,$$

where ε_{ijk} is the permutation tensor, show that in the limit $\theta \to 0$ the rotation matrix becomes:

$$R_{ij} = \delta_{ij} - \varepsilon_{ijk}\hat{\rho}_k\theta.$$

Hence show that the axis of the rotation described by the three independent components of ω_{kj} is parallel to $\operatorname{curl}\mathbf{u}$.

■

1.3.1 Normal strain and shear strain

The diagonal and off-diagonal components of the strain tensor of eqn.(1.8) are called *normal* and *shear* strains respectively. An example of a normal strain in two dimensions is illustrated in Fig.1.1(a), for the which the deformation tensor is:

$$\mathbf{F} = \begin{pmatrix} 1+\varepsilon & 0 \\ 0 & 1 \end{pmatrix}$$

and the corresponding strain tensor is

$$\mathbf{e} = \begin{pmatrix} \varepsilon & 0 \\ 0 & 0 \end{pmatrix}.$$

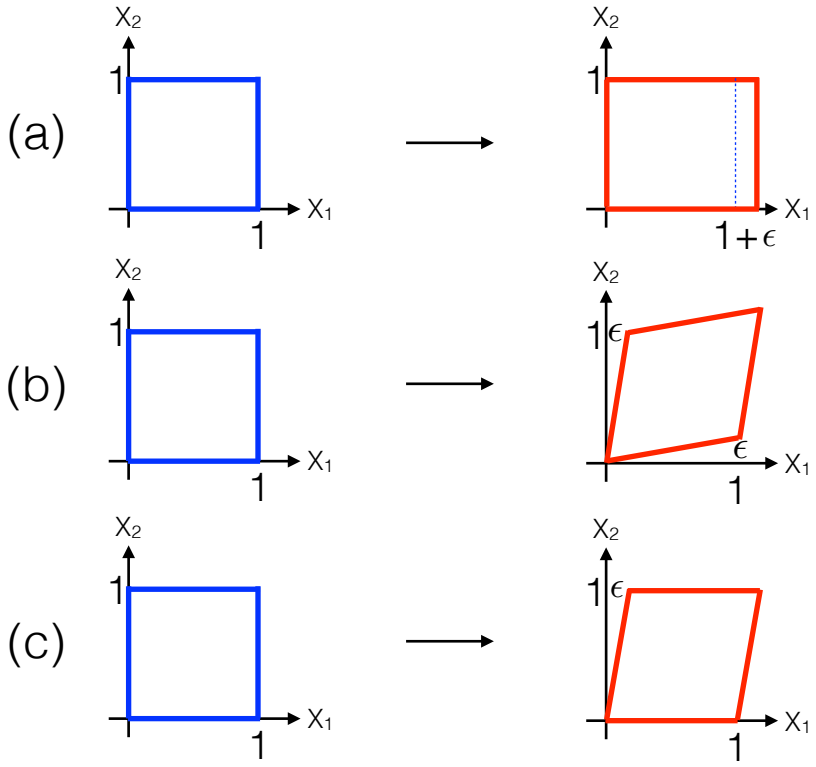

Figure 1.1: Illustrations in two dimensions of (a) normal strain along X_1, (b) pure shear strain and (c) simple shear strain. In each case the blue unit square on the left is deformed into the red shape on the right by the corresponding strain.

A shear strain arises when the displacement in a particular direction varies with a perpendicular distance. These two types of strain are illustrated in two dimensions in Fig.1.1.

Two common types of shear strain are a *pure shear* and a *simple shear*, both of which are illustrated in two dimensions in Fig.1.1. Fig.1.1(b) illustrates the pure shear described by the following deformation tensor:

$$\mathbf{F} = \begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix}$$

for which the corresponding strain tensor is

$$\mathbf{e} = \begin{pmatrix} 0 & \varepsilon \\ \varepsilon & 0 \end{pmatrix}.$$

The symmetric nature of the deformation tensor ensures it is a pure shear because no rotations are involved.

In contrast a simple shear involves a pure shear and a rotation. An example of a simple shear is illustrated in Fig.1.1(c) for which the deformation tensor is:

$$\mathbf{F} = \begin{pmatrix} 1 & \varepsilon \\ 0 & 1 \end{pmatrix}.$$

This may be decomposed into a pure shear strain of $\varepsilon/2$ and a rotation by $\theta = \varepsilon/2$ about an axis normal to the page:

$$\mathbf{F} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & \varepsilon/2 \\ \varepsilon/2 & 0 \end{pmatrix} + \begin{pmatrix} 0 & \varepsilon/2 \\ -\varepsilon/2 & 0 \end{pmatrix}.$$

Simple shears occur in *mechanical twinning*, which is a mechanism of deformation of many crystalline materials.

1.4 Closing remarks

The normal strain illustrated in Fig.1.1(a) changes the volume of the material. In contrast, the shear strains illustrated in Figs.1.1(b) and (c) do not change the volume, but unless the material is a liquid[2] there will be an elastic resistance to these deformations. Thomas Young FRS[3] was the first to consider shear as an elastic strain in 1807. He noticed that the elastic resistance of a body to shear is different from its resistance to extension or compression, but he did not introduce a separate elastic modulus to characterise the rigidity to shear. The famous 'Young's modulus' refers only to the rigidity of the material to elastic extension or compression. Love[4] commenting on Young's introduction of his modulus wrote:

This introduction of a definite physical concept, associated with the coefficient of elasticity which descends, as it were from a clear sky, on the reader of mathematical memoirs, marks an epoch in the history of the science.

We will come back to the moduli of elasticity in Chapter 3.

It should be noted that the concepts of the deformation tensor and the strain tensor rest on the existence of a reference state of the material where the deformation is sensibly regarded as zero. In a crystalline material the perfect crystal itself is a natural choice for the reference state. But in a glass or amorphous material there is no obvious choice of a reference state, and the concept of strain is much less useful. However, as we shall see in the next chapter the concept of stress is just as applicable in an amorphous material as it is in a crystal.

[2] Liquids do resist shear deformations in a time-dependent manner through their viscosities. But we are thinking here of the response of the material after a long period of time when any time-dependent relaxation processes have finished.

[3] For an engrossing biography of this exceptional polymath see *The last man who knew everything*, Andrew Robinson, One World: Oxford (2006).

[4] *A Treatise on the Mathematical Theory of Elasticity*, A. E. H. Love, Dover: New York (1944), p.4

1.5 Problem Set 1

1. Prove that the strain tensor of eqn.(1.8) satisfies the tensor transformation law under a rotation of the coordinate system.
2. Under a homogeneous strain the displacement of a point at $\mathbf{X}$ in the undeformed body is given by $\mathbf{u}(\mathbf{X}) = \mathbf{e} \cdot \mathbf{X}$, where $\mathbf{e}$ is a constant symmetric matrix, in which the elements are small compared to unity. Consider two points $\mathbf{X}^{(1)}$ and $\mathbf{X}^{(2)}$ in the undeformed body. Show that the change in the separation of the two points in the homogeneously deformed state to first order in the strain is given by $\left|\mathbf{X}^{(2)} - \mathbf{X}^{(1)}\right| l_i e_{ij} l_j$, where l_i is the unit vector $(X_i^{(2)} - X_i^{(1)})/\left|\mathbf{X}^{(2)} - \mathbf{X}^{(1)}\right|$.
3. Recall the eigenvectors of a symmetric matrix are orthogonal and the eigenvalues are real numbers. Consider a unit sphere $\mathbf{X}^T \cdot \mathbf{X} = 1$ embedded in a body before it is deformed. The body is subjected to a *homogeneous* strain $\mathbf{e}$. Show that the sphere becomes an ellipsoid with its axes aligned along the eigenvectors of the strain tensor. This ellipsoid is called the *strain ellipsoid*. If the eigenvalues of the strain tensor are λ_1, λ_2 and λ_3 determine the equation of the ellipsoid. Sketch the sphere and the ellipsoid, and for an arbitrarily chosen $\mathbf{X}$, show $\mathbf{x}$ and $\mathbf{u}$ in your sketch.
4. Prove that the trace of the strain tensor, e_{kk}, is invariant with respect to rotations of the coordinate system. Noting that it is dimensionless, like all strains, what is the physical meaning of this invariant quantity?

2. Stress

2.1 What is stress?

Imagine you are stretching an elastic band between your fingers by applying an equal and opposite tensile force F at either end. The elastic band has reached a new stable length and you keep your hands in a fixed position. There is no net force acting on any element of the elastic band. If that were not true the elastic band would not be in equilibrium and some further displacement would take place. But if you release the elastic band from one end it immediately shrinks back to its natural length.

We say 'the elastic band is under tension' to describe its state when it is stretched. If the stretched elastic band were cut anywhere between your fingers the tension would be released. The tension is transmitted across every transverse plane within the elastic band. The atoms on the left side of every transverse plane in the elastic band are exerting forces on the atoms of the right hand side. Conversely the atoms on the right hand side of every transverse plane are exerting forces on the left hand side. The resultant forces exerted by atoms on each side on the other side are equal and opposite when the elastic band is in equilibrium.

Suppose we stretch a thicker elastic band of the same material with the same force F. Obviously it will not stretch as much as the first elastic band. The task of transmitting the tension F across every transverse plane is shared by more atoms on either side of the plane. It follows that the area of the transverse plane is just as significant as the tension F in characterising the internal mechanical state of the elastic band. The concept of stress brings together the force F and the area of the plane on which it acts:

The stress acting on an element of area of a plane within a body is defined as the resultant force exerted by atoms on one side of the plane on atoms on the other side of the plane, where lines connecting those atoms pass through the element of area. The resultant force is divided by the area of the element through which it acts to yield the stress.

This is illustrated in Fig.2.1. This atomic-level definition of stress was developed by Cauchy and Saint-Venant in the 19th century before the existence of atoms was universally accepted, and long

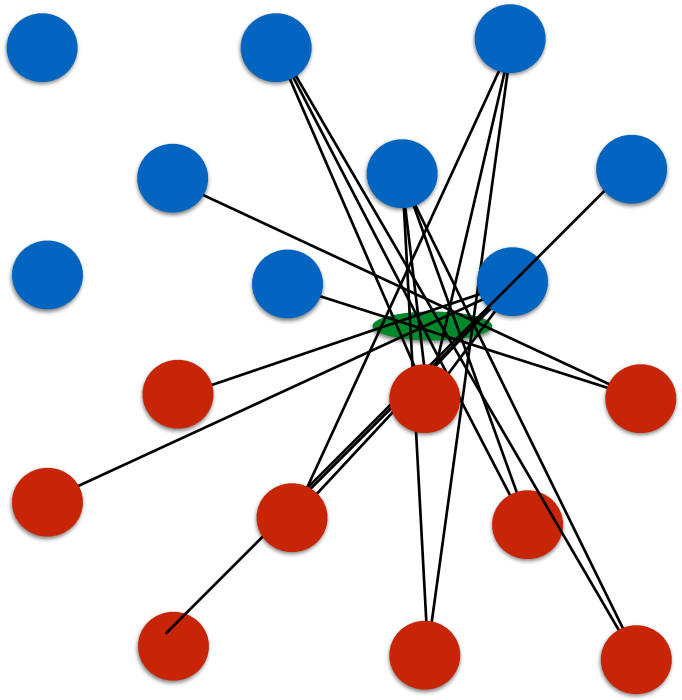

Figure 2.1: To illustrate the definition of stress. The green shaded area is a circle viewed in perspective. The stress acting on it is defined by those forces exerted by blue atoms on red atoms whose line of action passes through the green shaded area. The total force exerted through the shaded area becomes proportional to its size as its size increases. This is the continuum limit. Note that this definition does not assume atoms interact by pair potentials or even central force potentials. It is always possible to define the force exerted by one atom on another, as explained in the text.

before any real understanding of interatomic forces was developed [1]. Given the lack of knowledge about interatomic forces in the 1820s Cauchy developed a pragmatic continuum definition of stress, which is the way most engineers think about stress today. However, physicists have continued to develop atomic-level descriptions of stress up to the present day. In this chapter we will discuss both approaches.

The concept of pressure is closely related to stress: they both have dimensions of force per unit area (Newtons per square metre, which are called Pascals, in SI units). The key difference is that with pressure the force acting on the plane is always normal to the plane. With stress the force acting on the plane can be inclined to the plane normal, and can even be tangential to the plane. The tensorial nature of stress then becomes apparent because it depends on the direction of the resultant force *and* the direction of the normal to the plane on which it acts.

[1] see *History of strength of materials*, S P Timoshenko, Dover Publications: New York (1983), p.108

2.2 Cauchy's continuum stress tensor

Cauchy's definition of stress is simple but brilliant. He considered the force $\mathbf{f}$ per unit area acting on a plane in a continuum with unit normal $\hat{\mathbf{n}}$. Not knowing about the spatial range and nature of atomic interactions this force was assumed to have a negligible range and to exist only when the regions of the continuum on either side of the plane were in direct contact. If the plane is not flat its normal will vary with position. Apart from corners, where the normal changes discontinuously, it is always possible to define an infinitesimal element of area where the normal is constant. The concept of the continuum makes all this possible.

Consider a body in mechanical equilibrium but loaded in some arbitrary way, for example by forces applied to its surfaces. How do we calculate the infinitesimal force d$\mathbf{f}$ per unit area acting on an infinitesimal area dS with normal $\hat{\mathbf{n}}$ at any point inside the body? At first sight this might appear to be a hopeless task because there is an infinite number of plane normals. Cauchy showed it can be done by defining a tensor field of just six independent components, the stress field, inside the body.

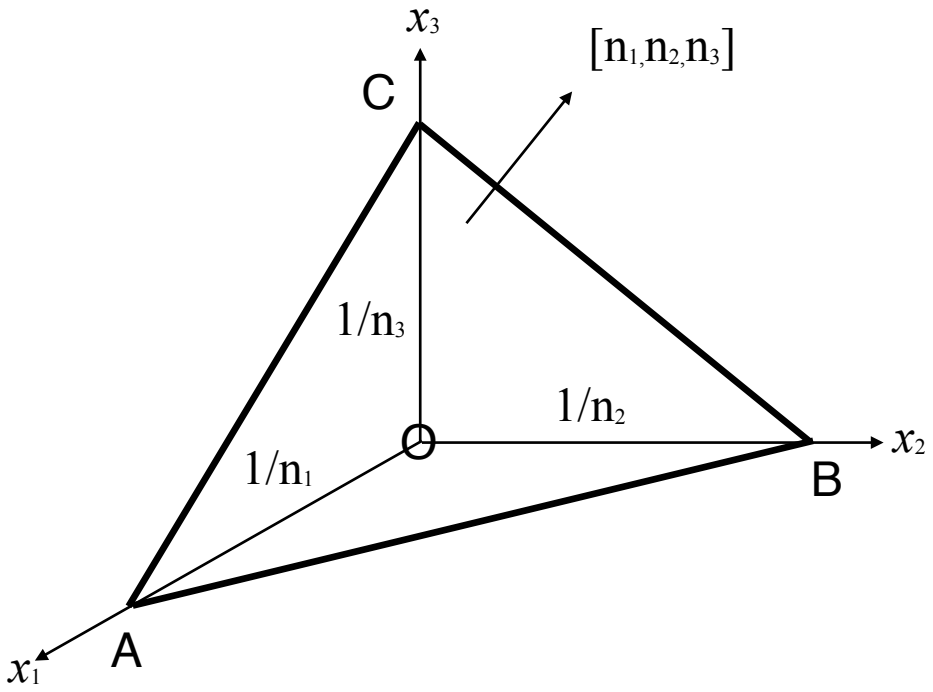

Figure 2.2: The triangle ABC has unit normal $\hat{\mathbf{n}} = [n_1, n_2, n_3]$ and area $1/(2n_1n_2n_3)$.

Define a right-handed global Cartesian coordinate system in the body, with axes x_1, x_2, x_3 and an arbitrary origin.

Consider the plane through the point $\mathbf{r}$ *with normal along the positive* x_j *direction. Let* dS *be an*

infinitesimal element of area of this plane at $\mathbf{r}$*. Then component* i *of the force per unit area acting on* $\mathrm{d}S$ *is the component* $\sigma_{ij}(\mathbf{r})$*, of the Cauchy stress tensor* $\boldsymbol{\sigma}$*.*

We will now show that the force per unit area acting on an infinitesimal element of area with an *arbitrary* outward unit normal $\hat{\mathbf{n}}$ at $\mathbf{r}$ can be expressed in terms of the stress tensor components $\sigma_{ij}(\mathbf{r})$. Let $\hat{\mathbf{n}} = [n_1, n_2, n_3]$ in this coordinate system. A plane with this normal has intercepts $1/n_1, 1/n_2, 1/n_3$ along the x_1, x_2, x_3 axes respectively, which is the plane ABC in Fig.2.2. The area of the triangle ABC is $1/(2n_1n_2n_3)$.

The plane ABC is parallel to the infinitesimal area element at $\mathbf{r}$. At equilibrium the net force acting on the body OABC must be zero. Component i of the force acting on the face OBC is $-\sigma_{i1} \times 1/(2n_2n_3)$, where the negative sign is because the outward normal to the face OBC is along $-x_1$, and $1/(2n_2n_3)$ is the area of OBC. Similarly, component i of the forces acting on the faces OAC and OAB are $-\sigma_{i2} \times 1/(2n_1n_3)$ and $-\sigma_{i3} \times 1/(2n_1n_2)$ respectively. If $\mathbf{f}$ is the force per unit area acting on the plane ABC then equilibrium of OABC requires:

$$\frac{f_i}{2n_1n_2n_3} - \frac{\sigma_{i1}}{2n_2n_3} - \frac{\sigma_{i2}}{2n_1n_3} - \frac{\sigma_{i3}}{2n_1n_2} = 0,$$

from which it follows that:

$$f_i = \sigma_{i1}n_1 + \sigma_{i2}n_2 + \sigma_{i3}n_3,$$

or,

$$f_i = \sigma_{ij}n_j. \tag{2.1}$$

This equation relates the force per unit area acting on a plane with normal $\hat{\mathbf{n}}$ in terms of the components of the stress tensor. In Exercise 2.2 the requirement that there is no torque acting on a volume element in the body leads to the condition $\sigma_{ij} = \sigma_{ji}$, i.e. the stress tensor is symmetric. Thus, there are only six independent components of the stress tensor. Eqn.(2.1) also shows that at equilibrium the forces per unit area acting on either side of a plane are equal and opposite because the sense of the plane normal reverses on either side. Finally, if σ_{ij} varies with position it becomes a stress field and the force per unit area acting on planes with a given normal also varies with position.

Exercise 2.1 Using eqn.2.1 prove that σ_{ij} satisfies the tensor transformation law under a rotation of the coordinate system. ∎

Exercise 2.2 (a) Sketch a cube of side length equal to unity with edges parallel to the axes Ox_1, Ox_2, Ox_3. Each face has unit area. As a result of a stress field each face experiences a force. On your sketch show the force acting on each face as an arrow and label it in terms of the components of the stress tensor. For example, on the face with normal parallel to the positive x_1 direction the three components of the force are $(\sigma_{11}, \sigma_{21}, \sigma_{31})$ with respect to the x_1, x_2 and x_3 axes respectively. But on the face with normal parallel to the negative x_1 axis the three components of the force are $(-\sigma_{11}, -\sigma_{21}, -\sigma_{31})$, so their arrows point in the opposite directions to those on the first face.
(b) By taking moments of the forces about the centre of the cube show that the condition for there to be no torque on a volume element we must have $\sigma_{ij} = \sigma_{ji}$. ∎

2.3 Normal stresses and shear stresses

We have seen that the force per unit area acting on an element of area of a plane may have components tangential to the plane as well as normal to it. The components parallel to the plane give rise to *shear* stresses, and they correspond to off-diagonal components of the stress tensor. The components normal to the plane are called *normal* stresses, and they correspond to diagonal components of the stress tensor. However, the designation of normal or shear stress may change under a rotation of the coordinate system, as shown in the next Exercise. Tensile and compressive stresses are normal stresses. Shear stresses arise in frictional sliding and they play a central role in plastic deformation of crystalline materials.

Exercise 2.3 A stress σ has the following representation in a Cartesian coordinate system $Ox_1x_2x_3$:

$$\sigma = \begin{pmatrix} -s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

When σ is represented in a rotated coordinate system $Ox_1'x_2'x_3'$, obtained by rotating Ox_1 and Ox_2 in a positive sense by $\pi/4$ about Ox_3, show that its matrix representation becomes:

$$\sigma = \begin{pmatrix} 0 & s & 0 \\ s & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

■

2.4 Stress at the atomic scale

After studying Cauchy's analysis of stress in terms of contact forces between elastic continua it may be surprising that the concept of stress can be developed at the atomic scale involving interactions between discrete atoms. An early treatment of stress at the atomic scale may be found in Note B, p.616 of Love's treatise of 1927, albeit for a perfect crystal. The treatment we shall give here is more general and applies to any system of interacting atoms, for which there is a model of atomic interactions.

Consider a cluster of atoms which may be subject to forces exerted by atoms outside the cluster. The cluster may be any size, from molecules to macroscopic components. The potential energy of the cluster is defined by the energy of interaction between all atoms in the cluster, and between atoms in the cluster and those outside it. Atoms in the cluster may be in a perfect crystal configuration, or a defective crystal or an amorphous state. Let $\mathbf{f}^{(n)}$ be the total force acting on atom n inside the cluster. This force comprises a sum of forces exerted by other atoms in the cluster, and by any atoms outside the cluster. Let $\mathbf{f}^{(m/n)}$ be the force exerted by atom m upon atom n, where atom m may be inside or outside the cluster. It follows that $\mathbf{f}^{(n)} = \sum_{m \neq n} \mathbf{f}^{(m/n)}$. It is shown below that it is always possible to decompose the total force on an atom into a sum of contributions from surrounding atoms.

Let the position of atom n be $\mathbf{X}^{(n)}$. Imagine all atoms inside the cluster are displaced by infinitesimal amounts $\delta\mathbf{X}^{(n)}$. Different atoms may be displaced in different directions. The change

in the total potential energy of the cluster is:

$$\begin{aligned}\delta V &= -\sum_n \mathbf{f}^{(n)} \cdot \delta \mathbf{X}^{(n)} \\ &= -\frac{1}{2}\sum_n \sum_{m\neq n} \mathbf{f}^{(m/n)} \cdot \delta\left(\mathbf{X}^{(n)} - \mathbf{X}^{(m)}\right),\end{aligned} \tag{2.2}$$

where the sum over n is taken over all atoms inside the cluster and the sum over m is taken over all atoms inside and outside the cluster. The factor of $\frac{1}{2}$ takes into account the sharing of the interaction between atoms n and m. Thus, eqn.(2.2) includes all interactions between atoms inside the cluster and between atoms inside and outside the cluster. The latter determine the forces exerted on the cluster by the surrounding medium.

Suppose the infinitesimal displacements of atoms are a result of the application of a homogeneous, infinitesimal strain δe_{ij} applied to all atoms inside and outside the cluster[2]. Since the applied strain is homogeneous and infinitesimal the change of $(X_i^{(n)} - X_i^{(m)})$ is $\delta e_{ij}(X_j^{(n)} - X_j^{(m)})$. Therefore the change in potential energy of the cluster in eqn.(2.2) becomes the following:

$$\delta V = -\frac{1}{2}\sum_n \sum_{m\neq n} f_i^{(m/n)} \delta e_{ij} \left(X_j^{(n)} - X_j^{(m)}\right). \tag{2.3}$$

We may use eqn.(2.3) to define atomic level stresses:

$$\delta V = \sum_n \Omega^{(n)} \sigma_{ij}^{(n)} \delta e_{ij}, \tag{2.4}$$

where $\Omega^{(n)}$ and and $\sigma_{ij}^{(n)}$ are the volume associated with atomic site n and the stress tensor associated with atomic site n inside the cluster. Comparing with eqn.(2.3) we obtain:

$$\sigma_{ij}^{(n)} = \frac{1}{2\Omega^{(n)}} \sum_{m\neq n} f_i^{(m/n)} \left(X_j^{(m)} - X_j^{(n)}\right) \tag{2.5}$$

where the sum over m is taken over atomic sites inside and outside the cluster. The atomic volume $\Omega^{(n)}$ may be defined by a Voronoi construction.

In eqn.(2.5) it is clear that even if the net force on an atom is zero it may still be in a state of stress. For example the atoms inside the cluster may be in a perfect crystal environment where each atom experiences zero net force, but the cluster is subjected to compression or tension through forces exerted by atoms outside the cluster that appear eqn.(2.3).

Even if the total force on an atom is not resolved analytically into a sum of contributions from surrounding atoms it is always possible to find the force $\mathbf{f}^{(m/n)}$ exerted by atom m upon atom n by the following procedure. After fixing the positions of all atoms in the configuration where we wish to determine $\mathbf{f}^{(m/n)}$ we remove atom n completely from the system. The positions of all other atoms are maintained constant. The change in the total force experienced by atom m following the removal of atom n is $-\mathbf{f}^{(n/m)}$, which is $\mathbf{f}^{(m/n)}$. In a self-consistent electronic structure calculation one would have to allow the electronic charge density to become self-consistent again after removing atom n, while maintaining fixed positions of all nuclei, before calculating the total force on atom m.

Provided no heat is exchanged between the cluster and its surroundings as a result of the application of the strain the change in the potential energy of the cluster is equal to the change in its

[2]When a homogeneous strain is applied to the cluster it also has to be applied to atoms outside the cluster, otherwise the changes of separation between atoms inside and outside the cluster will be incorrect because the cluster will have changed shape and/or volume but the surrounding medium will not have changed.

internal energy, δE. Then in a continuum approximation eqn.(2.4) becomes the following volume integral over the cluster:

$$\delta E = \sum_n \Omega^{(n)} \sigma_{ij}^{(n)} \delta e_{ij} \approx \int \mathrm{d}^3 X \, \sigma_{ij}(\mathbf{X}) \delta e_{ij}(\mathbf{X})$$

which leads to a new definition of stress in a continuum as the following functional derivative:

$$\sigma_{ij}(\mathbf{X}) = \frac{\delta E}{\delta e_{ij}(\mathbf{X})}, \tag{2.6}$$

where the variation is carried out adiabatically, i.e. at constant entropy. The definition of stress in eqn.(2.6) is based on the existence of a strain energy function describing the potential energy of the body as a function of a homogeneous elastic strain applied to it. The notion of a strain energy function was introduced by George Green (the mathematician and miller) in 1837 and put on a rigorous thermodynamic foundation by Sir William Thomson FRS (who became Lord Kelvin) in 1855. This definition of stress appears to be quite different from Cauchy's definition, but they are equivalent.

2.5 Invariants of the stress tensor

Let $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3$ be unit vectors along the right-handed Cartesian coordinate system x_1, x_2, x_3. Let $\hat{\mathbf{e}}'_1, \hat{\mathbf{e}}'_2, \hat{\mathbf{e}}'_3$ be unit vectors along the right-handed Cartesian coordinate system x'_1, x'_2, x'_3. The rotation matrix which rotates $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3$ into $\hat{\mathbf{e}}'_1, \hat{\mathbf{e}}'_2, \hat{\mathbf{e}}'_3$ has components $R_{ij} = (\hat{\mathbf{e}}'_i \cdot \hat{\mathbf{e}}_j)$, that is $\hat{\mathbf{e}}'_i = R_{ij}\hat{\mathbf{e}}_j$. Since stress is a second rank tensor it satisfies the following transformation law:

$$\sigma'_{jk} = R_{ji} R_{kp} \sigma_{ip}, \tag{2.7}$$

where $\boldsymbol{\sigma}'$ and $\boldsymbol{\sigma}$ are the matrix representations of the stress tensor in the primed and unprimed coordinate systems respectively.

Since the components of the matrix representing the stress tensor change under a coordinate transformation, individual stress tensor components have limited physical significance. However, there are three quantities that remain invariant under a rotation of the coordinate system, and they can be used to construct more physically significant quantities. The key to identifying invariants of the stress tensor is to recall that the eigenvalues do not depend on the choice of coordinate system. It follows that the cubic polynomial that defines the eigenvalues must have the same coefficients in all coordinate systems. Let the eigenvalues be s_1, s_2, s_3. When the coordinate system is aligned with the three eigenvectors of the matrix representing the stress tensor, the matrix becomes diagonal with s_1, s_2, s_3 along the leading diagonal. The cubic polynomial defining these eigenvalues is:

$$(s - s_1)(s - s_2)(s - s_3) = 0,$$

or

$$s^3 - (s_1 + s_2 + s_3)s^2 + (s_1 s_2 + s_2 s_3 + s_3 s_1)s - s_1 s_2 s_3 = 0.$$

It follows that the following three quantities are invariants:

$$\begin{aligned} I_1 &= s_1 + s_2 + s_3 \\ I_2 &= s_1 s_2 + s_2 s_3 + s_3 s_1 \\ I_3 &= s_1 s_2 s_3. \end{aligned} \tag{2.8}$$

Any quantity that may be expressed in terms of these invariants is also invariant. I_1 is the trace of the stress tensor, $\mathrm{Tr}\,\sigma$. The hydrostatic stress is defined as the average normal stress, which is $I_1/3$. The hydrostatic pressure, p, is the negative of the hydrostatic stress:

$$p = -\frac{1}{3}\mathrm{Tr}\,\sigma. \tag{2.9}$$

The second and third invariants may be expressed in any coordinate system as follows:

$$I_2 = \frac{1}{2}\left[(\mathrm{Tr}\,\sigma)^2 - \mathrm{Tr}\,\sigma^2\right] \tag{2.10}$$

$$I_3 = \frac{1}{6}\left[(\mathrm{Tr}\,\sigma)^3 + 2\mathrm{Tr}\,\sigma^3 - 3\,(\mathrm{Tr}\,\sigma)\left(\mathrm{Tr}\,\sigma^2\right)\right] \tag{2.11}$$

We note also that I_3 is the determinant of the stress tensor.

Stress invariants are useful for characterising the stress fields of defects in crystals, e.g. grain boundaries, because they are independent of the coordinate system. Strain energy functions are also often expressed in terms of stress invariants for similar reasons. Of course the strain tensor has equivalent invariants.

2.6 Shear stress on a plane and the Von Mises stress invariant

In the previous section we saw the hydrostatic stress is an invariant of the stress tensor. As the average of the three normal stresses in any coordinate system it is a scalar quantity which indicates the degree of compression or tension. It is useful to have another invariant quantity that measures the shear component of the stress tensor. This is somewhat more difficult because shear stresses, unlike hydrostatic stresses, depend on the normal of the plane where they act. Therefore, we begin this section by evaluating the magnitude of the shear stress acting on any plane for an arbitrary stress tensor.

Consider a stress tensor σ_{ij} with eigenvalues s_1, s_2, s_3 and corresponding unit eigenvectors $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3$. The eigenvectors form an orthonormal set, which defines the Cartesian coordinate system. Consider a plane with unit normal $\hat{\mathbf{n}} = n_i\hat{\mathbf{e}}_i$. The force per unit area acting on this plane is $\mathbf{f} = s_1 n_1 \hat{\mathbf{e}}_1 + s_2 n_2 \hat{\mathbf{e}}_2 + s_3 n_3 \hat{\mathbf{e}}_3$. The magnitude of the component of $\mathbf{f}$ along the normal $\hat{\mathbf{n}}$ is $f_n = \mathbf{f}\cdot\hat{\mathbf{n}} = s_1 n_1^2 + s_2 n_2^2 + s_3 n_3^2$. Therefore, the force per unit area normal to the plane is $\mathbf{f_n} = f_n\hat{\mathbf{n}}$. The force per unit area parallel to the plane is $\mathbf{f_p} = \mathbf{f} - (\mathbf{f}\cdot\hat{\mathbf{n}})\,\hat{\mathbf{n}}$. Thus,

$$\mathbf{f_p} = \left[s_1 n_1 - f_n n_1, s_2 n_2 - f_n n_2, s_3 n_3 - f_n n_3\right].$$

We may obtain a useful expression for the square of the magnitude of $\mathbf{f_p}$ as follows (the summation

convention is temporarily suspended to derive eqn.(2.12)):

$$\begin{aligned} f_p^2 &= \sum_i (s_i n_i - f_n n_i)^2 \\ &= \sum_i n_i^2 s_i^2 - \sum_i s_i n_i^2 \sum_j s_j n_j^2 \\ &= \sum_i n_i^2 s_i^2 \sum_j n_j^2 - \sum_i s_i n_i^2 \sum_j s_j n_j^2 \\ &= \sum_i \sum_j n_i^2 n_j^2 s_i^2 - n_i^2 n_j^2 s_i s_j \\ &= \frac{1}{2} \sum_i \sum_j n_i^2 n_j^2 (s_i^2 + s_j^2 - 2 s_i s_j) \\ &= \sum_{i<j} \sum_j n_i^2 n_j^2 (s_i - s_j)^2 \\ &= (s_1 - s_2)^2 n_1^2 n_2^2 + (s_2 - s_3)^2 n_2^2 n_3^2 + (s_3 - s_1)^2 n_3^2 n_1^2 \end{aligned} \tag{2.12}$$

If the stress is purely hydrostatic then, as expected, eqn.(2.12) shows the shear stress on all planes is zero. Consider the plane $n_3 = 0$ where $f_p^2 = (s_1 - s_2)^2 n_1^2 n_2^2$. This function is plotted in Fig.2.3, where it is seen that the maximum shear stress acts on planes at 45° to the principal stress directions $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$, with magnitude $|s_1 - s_2|/2$.

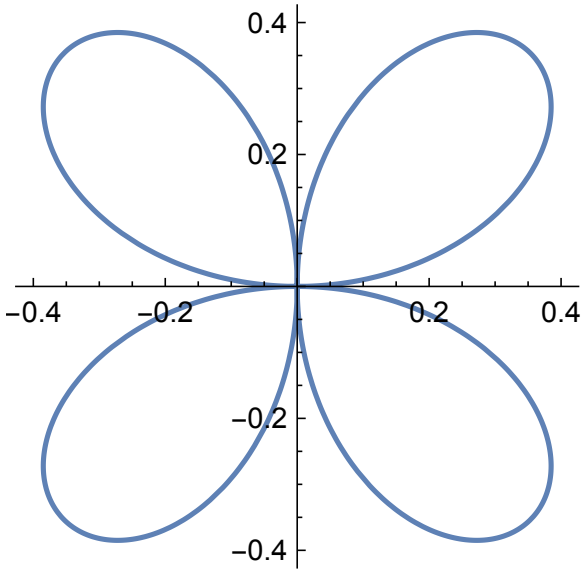

Figure 2.3: Plot of $f_p^2 = n_1^2 n_2^2$, where $n_1 = \cos\theta$ and $n_2 = \sin\theta$. The axes are aligned with the principal stress directions $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$. The horizontal axis is $\cos^2\theta \sin\theta$ and the vertical axis is $\sin^2\theta \cos\theta$, where $0 \le \theta \le 2\pi$.

Exercise 2.4 (a) Show that $f_p^2 = \hat{\mathbf{n}}^T \sigma^2 \hat{\mathbf{n}} - \left(\hat{\mathbf{n}}^T \sigma \hat{\mathbf{n}}\right)^2$, where $\hat{\mathbf{n}}^T$ is the transpose of $\hat{\mathbf{n}}$.
(b) Show that $\mathbf{f_p}$ is unaffected if σ_{ij} is replaced by $\sigma_{ij}^{(D)} = \sigma_{ij} - \frac{1}{3}(\mathrm{Tr}\,\sigma)\delta_{ij}$, where $\sigma^{(D)}$ is called the *deviatoric* stress.
(c) Using eqn.(2.12) show that the average value of f_p^2, where the averaging is over all orienta-

tions of $\hat{\mathbf{n}}$ on the surface of a unit sphere, is:

$$\begin{aligned} < f_p^2 > &= \frac{1}{15}\left((s_1-s_2)^2+(s_2-s_3)^2+(s_3-s_1)^2\right) \\ &= \frac{1}{15}\left(3\mathrm{Tr}\,\sigma^2-(\mathrm{Tr}\,\sigma)^2\right) \end{aligned} \tag{2.13}$$

■

The von Mises shear stress is a stress invariant that is used to characterise the degree of shear in a stress tensor. It is used for example as a yield criterion to decide whether the stress in a body enables plastic deformation to take place. It is defined by:

$$\sigma^{vM} = \frac{1}{\sqrt{2}}\sqrt{(s_1-s_2)^2+(s_2-s_3)^2+(s_3-s_1)^2} \tag{2.14}$$

The von Mises shear stress is $\sigma^{vM} = \sqrt{15/2}\times\sqrt{< f_p^2 >}$, and is therefore directly related to the average shear stress on a plane.

2.7 Mechanical equilibrium

We come now to one of the most important ideas in the continuum theory of elasticity, that of mechanical equilibrium. We have seen already that the stress tensor has to be symmetric if there are no torques acting. We consider now the equilibrium of a region $\mathscr{R}$ that experiences a force per unit volume $\mathbf{f}(\mathbf{X})$ within a body. This force may be gravitational for example, and it is called a *body force*. The continuum surrounding $\mathscr{R}$ distorts generating stresses that balance the net body force acting on $\mathscr{R}$. These stresses are transmitted to $\mathscr{R}$ through the surface $\mathscr{S}$ surrounding it.

Mechanical equilibrium requires that the total force acting on $\mathscr{R}$ is zero:

$$\int_{\mathscr{R}} f_i(\mathbf{X})\mathrm{d}V - \int_{\mathscr{S}} \sigma_{ij}n_j\mathrm{d}S = 0,$$

where n_j is component j of the *inward* pointing normal $\hat{\mathbf{n}}$ at the surface $\mathscr{S}$ of the region $\mathscr{R}$. The surface integral in this expression is the resultant force on $\mathscr{R}$ exerted by the continuum surrounding it. We normally use the *outward* normal in which case we must change the minus sign to a plus sign:

$$\int_{\mathscr{R}} f_i(\mathbf{X})\mathrm{d}V + \int_{\mathscr{S}} \sigma_{ij}n_j\mathrm{d}S = 0,$$

where n_j is now component j of the *outward* pointing normal $\hat{\mathbf{n}}$ at the surface $\mathscr{S}$ of the region $\mathscr{R}$. Using the divergence theorem this may be rewritten as:

$$\int_{\mathscr{R}} f_i(\mathbf{X}) + \sigma_{ij,j}\mathrm{d}V = 0,$$

where the comma denotes differentiation: $\partial Z/\partial X_j = Z_{,j}$, and $\sigma_{ij,j}$ is the divergence of the stress tensor. Since this balance of forces must hold for all regions $\mathscr{R}$ within the body we arrive at the following differential equations for mechanical equilibrium:

$$\sigma_{ij,j} + f_i = 0. \tag{2.15}$$

There are three equations here, one for each component i of the body force, and $\sigma_{ij,j}$ consists of three derivatives for each value of i. These equations are analogous to Poisson's equation in electromagnetism where the divergence of the electric displacement vector is the electric charge density, and electric charges are the sources of electric fields. In eqn.(2.15) body forces are the sources of stress fields. This is a concept which we will use throughout this book to relate the long-range elastic fields created by defects to the short-range forces exerted on atoms in the core of the defects.

Exercise 2.5 Consider the resultant torque T_i acting on a region $\mathscr{R}$ with surface $\mathscr{S}$ within a body. It is acted on by a distribution of body forces $f_i(\mathbf{x})$ within $\mathscr{R}$ and surface tractions[a] $t_i(\mathbf{x})$ on $\mathscr{S}$. If the region $\mathscr{R}$ is in mechanical equilibrium so that there is no resultant force acting upon it prove that the condition for the torque T_i to be zero is that the stress tensor is symmetric.

Hint
With respect to an arbitrary origin the torque acting on the region $\mathscr{R}$ is given by

$$\mathbf{T} = \int_{\mathscr{R}} \mathbf{x} \times \mathbf{f}\, \mathrm{d}V + \int_{\mathscr{S}} \mathbf{x} \times \mathbf{t}\, \mathrm{d}S.$$

Rewrite this equation in component form using suffix notation and use the divergence theorem to convert the surface integral into a volume integral. Then use the equilibrium condition $\sigma_{ij,j} + f_i = 0$ to simplify the terms and deduce the symmetry of the stress tensor as the condition for $T_i = 0$.

Why is the expression for the torque $\mathbf{T}$ independent of the choice of origin? ■

[a] A 'surface traction' is a force per unit area acting on a surface.

Exercise 2.6 In this question we use the equilibrium condition $\sigma_{ij,j} + f_i = 0$ to prove $\sigma_{ij} = \delta E / \delta e_{ij}(\mathbf{x})$.

Consider a region $\mathscr{R}$ with surface $\mathscr{S}$ within a body in which there is a distribution of body forces $f_i(\mathbf{x})$ within $\mathscr{R}$ and surface tractions $t_i(\mathbf{x})$ on $\mathscr{S}$. There is no net force acting on $\mathscr{R}$. Suppose an infinitesimal displacement field $\delta u_i(\mathbf{x})$ is applied to points within $\mathscr{R}$ and on $\mathscr{S}$, which does not disturb the equilibrium of the body. The work done δW by the body forces in $\mathscr{R}$ and surface tractions on $\mathscr{S}$ is:

$$\delta W = -\left\{ \int_{\mathscr{R}} f_i(\mathbf{x}) \delta u_i(\mathbf{x})\, \mathrm{d}V + \int_{\mathscr{S}} \sigma_{ij}(\mathbf{x}) \delta u_i(\mathbf{x}) n_j(\mathbf{x})\, \mathrm{d}S \right\},$$

where the normal vector in the surface integral points outwards. The corresponding change in the internal energy of the region $\mathscr{R}$ is $\delta E = -\delta W$. Thus,

$$\delta E = \int_{\mathscr{R}} f_i(\mathbf{x}) \delta u_i(\mathbf{x})\, \mathrm{d}V + \int_{\mathscr{S}} \sigma_{ij}(\mathbf{x}) \delta u_i(\mathbf{x}) n_j(\mathbf{x})\, \mathrm{d}S.$$

Use the divergence theorem to express the surface integral as a volume integral and simply the resulting terms using the equilibrium condition to show that:

$$\delta E = \int_{\mathscr{R}} \sigma_{ij} \delta u_{i,j} \mathrm{d}V.$$

Using the symmetry of the stress tensor show that this expression is equivalent to:

$$\delta E = \int_{\mathscr{R}} \sigma_{ij} \delta e_{ij} \mathrm{d}V.$$

Hence deduce $\sigma_{ij}(\mathbf{x}) = \delta E / \delta e_{ij}(\mathbf{x})$.

■

2.8 Problem Set 2

1. With respect to Cartesian axes x_1, x_2, x_3 a stress tensor σ is represented by the matrix

$$\sigma = \begin{pmatrix} 2 & 1 & 3 \\ 1 & 0 & -1 \\ 3 & -1 & 1 \end{pmatrix}$$

(a) Show that the force per unit area on the plane $2x_1 + x_2 - 2x_3 = 0$ is $\mathbf{f} = 1/3[-1,4,3]$.
(b) Show that the normal stress on this plane is $-4/9$.
(c) Show that the shear stress on this plane is $\sqrt{1962}/27$ and that it acts along the $[-1,40,19]$ direction.
(d) Show that the stress tensor when referred to a new set of Cartesian axes obtained by rotating the x_1 and x_3 axes by -45° about the positive x_2 axis (i.e. $[010]$) is given by:

$$\sigma = \frac{1}{2} \begin{pmatrix} 9 & 0 & -1 \\ 0 & 0 & -2\sqrt{2} \\ -1 & -2\sqrt{2} & -3 \end{pmatrix}$$

2. Consider an atomistic model in which the total potential energy is described by a sum of pair potentials:

$$E = \frac{1}{2} \sum_m \sum_{n \neq m} V(X^{(mn)})$$

where $X^{(mn)}$ is the separation $\left|\mathbf{X}^{(m)} - \mathbf{X}^{(n)}\right|$ between atoms m and n and $V(X)$ is a function of the separation between pairs of atoms, e.g. a Lennard-Jones potential. The factor of one half is to correct for the double counting in the sum over m and n. Show that the atomic level stress tensor at atom k is given by:

$$\sigma_{ij}^{(k)} = \frac{1}{2\Omega^{(k)}} \sum_{n \neq k} \left(\frac{\mathrm{d}V}{\mathrm{d}X}\right)_{X = X^{(nk)}} \frac{\left(X_i^{(n)} - X_i^{(k)}\right)\left(X_j^{(n)} - X_j^{(k)}\right)}{X^{(nk)}}.$$

3. (a) Using eqns.(2.14 and 2.13) show that

$$\sigma^{vM} = \frac{1}{\sqrt{2}}\sqrt{(\sigma_{11}-\sigma_{22})^2+(\sigma_{22}-\sigma_{33})^2+(\sigma_{33}-\sigma_{11})^2+6(\sigma_{12}^2+\sigma_{23}^2+\sigma_{31}^2)}. \quad (2.16)$$

(b) Show that the second invariant I_2 (see eqn.(2.10)) of the deviatoric stress tensor $(\sigma_{ij} - \delta_{ij}\sigma_{kk}/3)$ is directly proportional to the von Mises stress σ^{vM}, eqn.(2.13).

4. *This question is more advanced, but you are guided through each step. It is based on the work of the mathematician Walter Noll*[3].
We return to the definition of stress at the beginning of this chapter in terms of atomic interactions. Atoms are discrete objects and this poses a mathematical difficulty in applying the condition for mechanical equilibrium in a continuum embodied in eqn.(2.15). Noll's analysis overcomes this difficulty by replacing the discrete force that one atom exerts on another with a continuous force density $\mathbf{f}(\mathbf{x}',\mathbf{x})$ with units of force per unit volume squared. Then $\mathbf{f}(\mathbf{x}',\mathbf{x})\mathrm{d}V_{\mathbf{x}'}\mathrm{d}V_{\mathbf{x}}$ is the force that a volume element $\mathrm{d}V_{\mathbf{x}'}$ at $\mathbf{x}'$ exerts on a volume element $\mathrm{d}V_{\mathbf{x}}$ at $\mathbf{x}$. Notice that $\mathbf{f}(\mathbf{x}',\mathbf{x}) = -\mathbf{f}(\mathbf{x},\mathbf{x}')$. If the stress tensor at $\mathbf{x}$ is $\sigma_{ij}(\mathbf{x})$ then Noll proves that:

$$\sigma_{ij,j}(\mathbf{x}) = \int_V f_i(\mathbf{x}',\mathbf{x})\mathrm{d}V_{\mathbf{x}'} \quad (2.17)$$

This is the resultant force acting on a volume element at $\mathbf{x}$ arising from the surrounding medium. It is important to recognise that although $\mathbf{f}(\mathbf{x}',\mathbf{x})$ depends only on $\mathbf{x}'$ and $\mathbf{x}$ this does not amount to an assumption of a description of the interaction as a pair potential. In other words $\mathbf{f}(\mathbf{x}',\mathbf{x})$ may depend on the *environments* of $\mathbf{x}'$ and $\mathbf{x}$. It is also *not* necessarily the case that the force $\mathbf{f}(\mathbf{x}',\mathbf{x})$ is parallel to $\mathbf{x}-\mathbf{x}'$.

Following Noll we will show that:

$$\sigma_{ij}(\mathbf{x}) = \frac{1}{2}\int_S \mathrm{d}\Omega_m \int_{r=0}^{\infty} \mathrm{d}r\, r^2 \int_{\alpha=0}^{1} \mathrm{d}\alpha\, f_i(\mathbf{x}+\alpha r\hat{\mathbf{m}}, \mathbf{x}-(1-\alpha)r\hat{\mathbf{m}}) r m_j \quad (2.18)$$

where $\mathrm{d}\Omega_m$ is a solid angle element centred on the direction $\hat{\mathbf{m}}$, and the integral over S is over the unit sphere centred at $\mathbf{x}$. The magnitude of the vector $\mathbf{r}$ is r. The function $f_i(\mathbf{x}+\alpha r\hat{\mathbf{m}}, \mathbf{x}-(1-\alpha)r\hat{\mathbf{m}})$ is the force exerted by a volume element at $\mathbf{x}+\alpha r\hat{\mathbf{m}}$ on the volume element at $\mathbf{x}-(1-\alpha)r\hat{\mathbf{m}}$, where these volume elements are separated by r at all values of $0 \le \alpha \le 1$. As α varies between 0 and 1 in the third integral the forces of interaction that pass through $\mathbf{x}$ between all points separated by r along the direction $\hat{\mathbf{m}}$ are included. In the second integral r ranges over all possible separations, and in the first integral all possible directions $\hat{\mathbf{m}}$ are considered. In this way all forces of interaction that pass through $\mathbf{x}$ between points on either side of $\mathbf{x}$ contribute to the stress, in accord with the italicised definition of stress in section 2.1. Each interaction is counted twice, and this is corrected by the factor of one half. The reason for the final factor rm_j will become clear shortly.

[3] see `http://www.math.cmu.edu/~wn0g/`. On this web-site there are many fascinating articles, including a very thought-provoking one entitled *On the role of the professor*.

To prove eqn.(2.18) we show that it satisfies eqn.(2.17). Let $\mathbf{u} = \mathbf{x} + \alpha r\hat{\mathbf{m}}$ and $\mathbf{v} = \mathbf{x} - (1-\alpha)r\hat{\mathbf{m}}$. Show that:

$$\frac{\partial f_i}{\partial x_j} = \frac{\partial f_i}{\partial u_j} + \frac{\partial f_i}{\partial v_j}.$$

Using the chain rule show that:

$$\begin{aligned} \frac{\partial f_i}{\partial \alpha} &= \left(\frac{\partial f_i}{\partial u_j} + \frac{\partial f_i}{\partial v_j} \right) r m_j \\ &= \frac{\partial f_i}{\partial x_j} r m_j \end{aligned}$$

Using these results obtain eqn.(2.17).

Observations

- The stress in eqn.(2.18) has the correct units, i.e. force per unit area.
- The stress at $\mathbf{x}$ is attributed to forces that act not only on $\mathbf{x}$ but also through $\mathbf{x}$.
- Eqn.(2.18) is a continuum version of the discrete atomic-level stress tensor of eqn.(2.5).
- In eqn.(2.17) the force flux is inward towards the point $\mathbf{x}$: it is the resultant force the surrounding medium exerts on the point $\mathbf{x}$. If this resultant force is not zero then mechanical equilibrium requires there is an equal and opposite body force acting at $\mathbf{x}$. The body force exerts itself at $\mathbf{x}$ outwards on the surrounding medium. The right hand side of eqn.(2.17) is therefore equal and opposite to the body force at $\mathbf{x}$.

3. Hooke's law and elastic constants

3.1 Generalised Hooke's law: elastic constants and compliances

Robert Hooke (1635-1703) was one of the most versatile and accomplished experimentalists of all time[1]. He was appointed 'Curator of Experiments' in the Royal Society in 1662, two years after the Society was formed, a post he held for 40 years until his death in 1703. He was elected to a Fellowship of the Royal Society in 1663 at the age of 28.

The modern form of the law which takes his name is that the stress tensor is proportional to the strain tensor, and conversely the strain tensor is proportional to the stress tensor. Since both stress and strain are second rank tensors the proportionality constants are fourth rank tensors:

$$\sigma_{ij} = c_{ijkl}\, e_{kl} \tag{3.1}$$

$$e_{ij} = s_{ijkl}\, \sigma_{kl}, \tag{3.2}$$

where c_{ijkl} is called the elastic stiffness tensor, or elastic constant tensor, and s_{ijkl} is called the elastic compliance tensor. By substituting eqn.(3.2) into eqn.(3.1), and noting that the stress and strain tensors are symmetric, it is seen that the elastic constant and compliance tensors are related as follows:

$$c_{ijkl}\, s_{klmn} = \frac{1}{2}\left(\delta_{im}\delta_{jn} + \delta_{in}\delta_{jm}\right). \tag{3.3}$$

Exercise 3.1 Verify eqn.(3.3).
■

The direct proportionality between stress and strain is the basis of *linear* elasticity. Hooke's 'law' is an approximation because nonlinear terms become significant as the magnitude of the strain increases, but are neglected in the linear theory. Physically, stiffer bonds between atoms lead to

[1] see *The curious life of Robert Hooke* by Lisa Jardine (2003).

larger elastic constants and smaller elastic compliances. Thus, in diamond, which is a very stiff insulator, c_{1111} is 1,079 GPa, while in lead, which is a soft metal, it is 49.66 GPa. In most metals the elastic constants are of order 10^{11} GPa. One GPa (gigapascal) is 10^9 Pa, and 1 Pa = 1 N m^{-2} = 1 J m^{-3}; 1 GPa $\approx 6.24 \times 10^{-3}$ eV Å^{-3}.

3.2 The maximum number of independent elastic constants in a crystal

Since the elastic constant tensor is a fourth rank tensor it appears at first sight that there are $3^4 = 81$ independent elastic constants. If that were true the theory of elasticity would be much less useful because it would require the measurement of 81 material parameters. Symmetry enables the number of independent elastic constants to be reduced to a much more manageable number. The smallest number of independent elastic constants is just two, and this is the case in an elastically isotropic material like rubber. In cubic crystals there are just three independent elastic constants and in hexagonal crystals five. Since these restrictions are determined by symmetry they apply to the elastic compliance tensor in the same way as they do to the elastic constant tensor.

The largest number of independent elastic constants in any material is 21. This is the case in a triclinic crystal where there are no rotational symmetries in the point group. The first reduction is achieved by enforcing the symmetry of the stress and strain tensors: $\sigma_{ij} = \sigma_{ji}$, $e_{kl} = e_{lk}$. Therefore we must have $c_{ijkl} = c_{jikl} = c_{ijlk} = c_{jilk}$. The second reduction is more subtle and was first shown by George Green when he introduced the strain energy function, or elastic energy density.

3.2.1 The elastic energy density

In linear elasticity the elastic energy density is given by:

$$\begin{aligned} E &= \frac{1}{2}\sigma_{ij}e_{ij} \\ &= \frac{1}{2}c_{ijkl}e_{ij}e_{kl}. \end{aligned} \tag{3.4}$$

This expression comes from integrating $\mathrm{d}E = \sigma_{ij}\mathrm{d}e_{ij}$ with respect to strain from $e_{ij} = 0$ to the final strain and using Hooke's law to express stress in terms of strain. The factor of one half is a consequence of the linear relationship between stress and strain. The elastic energy density has units of J m^{-3}, the same as the elastic constants. The total elastic energy is then the integral of the elastic energy density over the volume of the body.

The elastic constants are second derivatives of the elastic energy density with respect to strain. For example, consider the terms involving the product $e_{12}e_{32}$. Since $e_{12} = e_{21}$ and $e_{32} = e_{23}$ we cannot vary e_{12} and e_{32} without also varying e_{21} and e_{23}. Therefore, there are four terms in the elastic energy density to consider: $\frac{1}{2}\left[c_{1232}e_{12}e_{32} + c_{2132}e_{21}e_{32} + c_{1223}e_{12}e_{23} + c_{2132}e_{21}e_{32}\right]$. We have already seen that $c_{1232} = c_{2132} = c_{1223} = c_{2132}$. Therefore these 4 terms amount to $2c_{1232}\ e_{12}\ e_{32}$, and

$$c_{1232} = \frac{1}{2}\frac{\partial^2 E}{\partial e_{12}\partial e_{32}}.$$

But there are also four terms in the elastic energy density involving the product $e_{32}e_{12}$. They amount to $2c_{3212}\ e_{32}\ e_{12}$, and

$$c_{3212} = \frac{1}{2}\frac{\partial^2 E}{\partial e_{32}\partial e_{12}}.$$

Green argued that the order of differentiation in these two second derivatives cannot matter. It follows that $c_{1232} = c_{3212}$. More generally,

$$c_{ijkl} = c_{klij}. \tag{3.5}$$

Thus the elastic constant tensor displays the following symmetries in all materials:

$$c_{ijkl} = c_{jikl} = c_{ijlk} = c_{jilk} = c_{klij} = c_{lkij} = c_{klji} = c_{lkji}. \tag{3.6}$$

There are six independent $\{ij\}$ and $\{kl\}$ combinations: 11, 22, 33, 23, 13 and 12. The symmetry embodied in eqn.(3.5) reduces the number of independent elastic constants from $6 \times 6 = 36$ to $6+5+4+3+2+1 = 21$. This was first demonstrated by Green in 1837[2]. Any further reduction in the number of independent elastic constants depends on the point group symmetry of the material.

3.2.2 Matrix notation

Green's analysis above suggests that Hooke's law can be expressed in a convenient matrix form where each index signifies two indices in the tensor form of the equation:

$$11 \to 1,\ 22 \to 2,\ 33 \to 3,\ 23 \text{ or } 32 \to 4,\ 13 \text{ or } 31 \to 5,\ 12 \text{ or } 21 \to 6.$$

For example, $\sigma_{31} \to \sigma_5$ and $c_{1232} \to c_{64}$. Hooke's law may then be written in the following matrix form:

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{21} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{31} & c_{32} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{41} & c_{42} & c_{43} & c_{44} & c_{45} & c_{46} \\ c_{51} & c_{52} & c_{53} & c_{54} & c_{55} & c_{56} \\ c_{61} & c_{62} & c_{63} & c_{64} & c_{65} & c_{66} \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \\ e_6 \end{bmatrix} \tag{3.7}$$

Now we see explicitly that there are just 21 independent components of the matrix $\mathbf{c}$. Let us compare this equation with the tensor form of Hooke's law, eqn.(3.1). For example, consider σ_{11} in eqn.(3.1):

$$\sigma_{11} = c_{1111}e_{11} + c_{1122}e_{22} + c_{1133}e_{33} + 2c_{1123}e_{23} + 2c_{1113}e_{13} + 2c_{1112}e_{12}.$$

This has to be equivalent to σ_1 in eqn.(3.7) to

$$\sigma_1 = c_{11}e_1 + c_{12}e_2 + c_{13}e_3 + c_{14}e_4 + c_{15}e_5 + c_{16}e_6.$$

For these two expressions to be equivalent we must have:

$$\begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \\ e_6 \end{bmatrix} = \begin{bmatrix} e_{11} \\ e_{22} \\ e_{33} \\ 2e_{23} \\ 2e_{13} \\ 2e_{12} \end{bmatrix}$$

[2] G. Green, Transactions of the Cambridge Philosophical Society, **7**, 1 (1839), available online at `https://archive.org/details/transactionsofca07camb`

Note the factors of 2 for the off-diagonal elements of the strain tensor.

It is important to recognise that $\boldsymbol{\sigma}, \mathbf{c}$ and $\mathbf{e}$ in eqn.(3.7) are *not* tensors because they do not transform according to the tensor transformation law under a rotation. They are merely a convenient way of writing the tensor relationship in eqn.(3.1) as a matrix equation. This highlights the difference between tensors and their representations as matrices.

3.3 Transformation of the elastic constant tensor under a rotation

We have seen that since stress and strain are second rank tensors they are related in Hooke's law by a fourth rank tensor, which is either the elastic constant tensor or the elastic compliance tensor. For a rotation of the Cartesian coordinate system defined as in eqn.(2.7) the elastic constant tensor transforms as follows:

$$c'_{ijkl} = R_{im}R_{jn}R_{kp}R_{lq}c_{mnpq} \tag{3.8}$$

We shall use this transformation to reduce the number of independent elastic constants to less that 21 when $\mathbf{R}$ represents a rotational symmetry of the material.

We note a further useful transformation property. If (x'_1, x'_2, x'_3) and (x_1, x_2, x_3) are the coordinates of a point in the rotated and unrotated coordinate systems respectively then

$$x'_i x'_j x'_k x'_l = R_{im}R_{jn}R_{kp}R_{lq}x_m x_n x_p x_q. \tag{3.9}$$

This equation shows that the elastic constant tensor c_{mnpq} transforms under a rotation in exactly the same way as the product of coordinates $x_m x_n x_p x_q$. We shall make use of this observation quite extensively below.

3.3.1 Neumann's principle

This is a fundamental principle that relates the symmetry displayed by a physical property of a crystal to the point group symmetry of the crystal. It is arguably the most fundamental structure-property relationship in the whole of materials science. It was formulated by Franz Neumann (1798-1895) and first appeared in print in 1885[3]. Here is the how International Union of Crystallography states the principle:

The symmetry elements of any physical property of a crystal must include all the symmetry elements of the point group of the crystal.

Mathematically, Neumann's principle means that the tensor representing any physical property is invariant with respect to every symmetry operation of the crystal. This means that when we transform the elastic constant tensor according to eqn.(3.8), with the rotation $\mathbf{R}$ being one of the symmetry rotations of the crystal, we must obtain an elastic constant tensor that is equivalent to the elastic constant tensor before the transformation was applied.

Note the word 'include' in Neumann's principle: the physical property may display more symmetry than the point group of the crystal. For example, the diffusivity tensor in a cubic crystal is isotropic, so that it displays the symmetry of a sphere in 3D, i.e. the rotation group SO(3), which is obviously more symmetric than a cube or octahedron or tetrahedron. The elastic constant tensor always displays inversion symmetry because if a homogeneous stress and strain

[3] F. E. Neumann, *Vorlesungen über die Theorie der Elastizität der festen Körper und des Lichtäthers*, (1885), ed. O. E. Meyer. Leipzig, B. G. Teubner-Verlag

were inverted through any centre no change would be apparent in the elastic properties since a state of homogeneous stress or strain is centrosymmetrical[4]. This remains true even in a crystal that does not display inversion symmetry in its point group. All point group operations are either rotations or rotations combined with an inversion (e.g. mirror planes are 2-fold rotations followed (or preceded) by an inversion). Since the elastic constant tensor already displays inversion symmetry it is necessary to ask how it transforms under only the rotational symmetries of the point group. Eleven of the 32 point groups contain only rotational symmetries, and they are known as the proper groups, or enantiomorphous groups. They are the point groups that determine the numbers of independent elastic constants in all 32 point groups.

3.4 Isotropic materials

An elastically isotropic material is one in which the elastic constants do not depend on direction in the material: they have the symmetry of SO(3). Good examples of isotropic materials are rubber, glass, liquids and amorphous materials.

If c_{ijkl} is the same in all directions then $c_{ijkl} = \langle c_{ijkl} \rangle$ where $\langle \dots \rangle$ means an average taken over all radial directions within a sphere. It follows from eqn.(3.9) that $\langle c_{ijkl} \rangle$ is proportional to $\langle x_i x_j x_k x_l \rangle$, where x_i are the coordinates of a point on the surface of the unit sphere, with respect to an origin at its centre. Temporarily suspending the summation convention on repeated indices we find:

$$\begin{aligned} < x_i x_j x_k x_l > &= < x_i^2 x_k^2 > \delta_{ij}\delta_{kl}(1-\delta_{ik}) \\ &\quad + < x_i^2 x_j^2 > \delta_{ik}\delta_{jl}(1-\delta_{ij}) + < x_i^2 x_k^2 > \delta_{il}\delta_{jk}(1-\delta_{ik}) + < x_i^4 > \delta_{ij}\delta_{jk}\delta_{kl} \\ &= \frac{1}{15}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ &\quad + \frac{1}{15}(3\delta_{ij}\delta_{ik}\delta_{il} - \delta_{ij}\delta_{kl}\delta_{ik} - \delta_{ik}\delta_{jl}\delta_{ij} - \delta_{il}\delta_{jk}\delta_{ik}) \\ &= \frac{1}{15}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \end{aligned} \tag{3.10}$$

where $< x_i^2 x_j^2 >= \frac{1}{15}(i \neq j), < x_i^4 >= \frac{1}{5}$ have been used. It follows that an isotropic elastic constant tensor has the following form:

$$c_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu\delta_{ik}\delta_{jl} + \mu'\delta_{il}\delta_{jk},$$

where λ, μ and μ' are constants.

Since $c_{ijij} = c_{ijji}$ (no summation) we must have $\mu = \mu'$. Therefore there are just two independent elastic constants in an isotropic material:

$$c_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right). \tag{3.11}$$

λ is called Lamé's first constant[5], and μ is sometimes called Lamé's second constant but more commonly the shear modulus.

Exercise 3.2 Derive eqn.(3.10) in detail. ∎

[4] J.F Nye, *Physical properties of crystals*, Oxford University Press (1957), p.21. This book is highly recommended. There have been others after it covering much the same ground, but none have been clearer than Nye's book.

[5] named after Gabriel Lamé (1795-1870)

Exercise 3.3 Verify that $c_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)$ is invariant when it substituted into eqn.(3.8) for any rotation $\mathbf{R}$.
■

When we substitute the isotropic elastic constants, eqn.(3.11), into Hooke's law, eqn,(3.1), we obtain the following equations:

$$\begin{aligned}
\sigma_{11} &= 2\mu e_{11} + \lambda(e_{11} + e_{22} + e_{33}) \\
\sigma_{22} &= 2\mu e_{22} + \lambda(e_{11} + e_{22} + e_{33}) \\
\sigma_{33} &= 2\mu e_{33} + \lambda(e_{11} + e_{22} + e_{33}) \\
\sigma_{23} &= 2\mu e_{23} \\
\sigma_{13} &= 2\mu e_{13} \\
\sigma_{12} &= 2\mu e_{12},
\end{aligned} \tag{3.12}$$

where we recognise $e_{kk} = e_{11} + e_{22} + e_{33}$ as the dilation $\Delta V/V$. Thus $c_{11} = 2\mu + \lambda$, $c_{12} = \lambda$ and $c_{44} = \mu$. Therefore in an isotropic material we have

$$A = \frac{2c_{44}}{c_{11} - c_{12}} = 1 \tag{3.13}$$

This is called the anisotropy ratio, about which we will say more in the context of cubic crystals where $A \neq 1$.

To relate λ and μ to Young's modulus Y consider a tensile test where a sample is loaded in tension along the x_3 axis and no constraints or loads are applied along x_1 and x_2. There are no shear stresses and equations (3.12) become:

$$\begin{aligned}
0 &= 2\mu e_{11} + \lambda(e_{11} + e_{22} + e_{33}) \\
0 &= 2\mu e_{22} + \lambda(e_{11} + e_{22} + e_{33}) \\
\sigma_{33} &= 2\mu e_{33} + \lambda(e_{11} + e_{22} + e_{33}).
\end{aligned}$$

Solving these equations for e_{11}, e_{22} and e_{33} we obtain $e_{11} = e_{22} = -\lambda\sigma_{33}/\{2\mu(2\mu + 3\lambda)\}$ and $e_{33} = 2(\mu + \lambda)\sigma_{33}/\{2\mu(2\mu + 3\lambda)\}$. From these relations we deduce the following:

$$Y = \frac{\mu(2\mu + 3\lambda)}{\mu + \lambda} \tag{3.14}$$

$$\nu = -\frac{e_{11}}{e_{33}} = \frac{\lambda}{2(\mu + \lambda)} \tag{3.15}$$

$$\mu = \frac{Y}{2(1 + \nu)} \tag{3.16}$$

$$\lambda = \frac{2\mu\nu}{1 - 2\nu}, \tag{3.17}$$

where ν is called Poisson's ratio. Poisson's ratio is the ratio of the contraction in the lateral x_1 and x_2 directions to the tensile strain along x_3. Most materials contract along the lateral directions when they are stretched, and expand along the lateral directions when they are compressed. Materials that

do the opposite are called 'auxetic', and they have negative Poisson's ratios. In terms of the Young's modulus and Poisson's ratio the strains may be expressed in terms of the stresses as follows:

$$\begin{aligned}
e_{11} &= \frac{\sigma_{11}}{Y} - \frac{\nu\sigma_{22}}{Y} - \frac{\nu\sigma_{33}}{Y} \\
e_{22} &= \frac{\sigma_{22}}{Y} - \frac{\nu\sigma_{11}}{Y} - \frac{\nu\sigma_{33}}{Y} \\
e_{33} &= \frac{\sigma_{33}}{Y} - \frac{\nu\sigma_{11}}{Y} - \frac{\nu\sigma_{22}}{Y} \\
e_{23} &= \frac{1+\nu}{Y}\sigma_{23} = \frac{\sigma_{23}}{2\mu} \\
e_{13} &= \frac{1+\nu}{Y}\sigma_{13} = \frac{\sigma_{13}}{2\mu} \\
e_{12} &= \frac{1+\nu}{Y}\sigma_{12} = \frac{\sigma_{12}}{2\mu}
\end{aligned} \tag{3.18}$$

Another commonly used elastic constant is the bulk modulus, B. This relates the hydrostatic pressure $p = -\mathrm{Tr}\sigma/3$ to the dilation $\Delta V/V = \mathrm{Tr}e$:

$$p = -B\frac{\Delta V}{V}. \tag{3.19}$$

Using equations (3.12) it is deduced that:

$$B = \frac{1}{3}(2\mu + 3\lambda) = \frac{2\mu(1+\nu)}{3(1-2\nu)} \tag{3.20}$$

It is stressed that in isotropic elasticity only two of the Young's modulus Y, the shear modulus μ, Poisson's ratio ν, the bulk modulus B and Lamé's first constant λ are independent.

Exercise 3.4 (a) Why must the value of ν always be between -1 and $\frac{1}{2}$?
(b) What do these two limits correspond to physically?
■

Exercise 3.5 Show that in an isotropic medium Hooke's law may be expressed in the following equivalent ways:

$$\begin{aligned}
\sigma_{ij} &= 2\mu e_{ij}^{(d)} + \delta_{ij} B e_{kk} \\
e_{ij} &= \frac{1}{2\mu}\sigma_{ij}^{(d)} + \delta_{ij}\frac{\sigma_{kk}}{9B}
\end{aligned}$$

where $e_{ij}^{(d)}$ and $\sigma_{ij}^{(d)}$ are the deviatoric strain and stress tensors. By introducing the deviatoric stress and strain tensors we see a clear separation between shear and dilational contributions, involving the shear modulus and bulk modulus respectively, to the total stress and strain tensors.
■

Exercise 3.6 (a) By orienting the axes along the eigenvectors of the stress tensor show that the elastic energy density in an isotropic medium may be expressed as follows:

$$E = \frac{1}{2Y}\left(s_1^2 + s_2^2 + s_3^2 - 2\nu\left(s_1 s_2 + s_2 s_3 + s_3 s_1\right)\right),$$

where s_i are the eigenvalues of the stress tensor.
(b) Show that the elastic energy density may be expressed as:

$$E = \frac{I_1^2}{18B} + \frac{I_1^2 - 3I_2}{6\mu} = \frac{p^2}{2B} + \frac{\left(\sigma^{vM}\right)^2}{6\mu}$$

where I_1 and I_2 are the first and second invariants of the stress tensor, p is the hydrostatic pressure and σ^{vM} is the von Mises shear stress given by eqn.(2.14). We see here that the elastic energy density in an isotropic medium also separates into dilational and shear contributions. ■

3.5 Anisotropic materials

There are no crystalline materials that are exactly elastically isotropic, but tungsten is almost isotropic. In this section we will illustrate how point group symmetry is used to reduce the number of independent elastic constants from 21 in a crystal. As an example we will show there are 3 independent elastic constants in cubic crystals.

3.5.1 Cubic crystals

In this section we will make use of the observation in eqn.(3.9) that the elastic constant tensor c_{mnpq} transforms under a rotation in exactly the same way as the product of coordinates $x_m\, x_n\, x_p\, x_q$.

Cubic crystals are defined by four 3-fold rotational symmetry axes along $\langle 111\rangle$ directions. These rotational symmetries generate a further three 2-fold rotation axes along $\langle 100\rangle$. In this way we obtain the cubic point group '23' in Hermann-Mauguin notation or T in Schönflies notation.

Rotating the coordinate axes by π about $[100]$ results in $x_1' = x_1, x_2' = -x_2, x_3' = -x_3$. Therefore the following eight elastic constants must be zero because they are equal to their own negative under this rotation: $c_{1112} = c_{16}, c_{1113} = c_{15}, c_{2212} = c_{26}, c_{2213} = c_{25}, c_{3312} = c_{36}, c_{3313} = c_{35}, c_{2312} = c_{46}, c_{2313} = c_{45}$, where we are specifying the 4-index tensor component and its corresponding element of the 6×6 matrix in eqn.(3.7).

Similarly rotating the coordinate axes by π about $[010]$ results in $x_1' = -x_1, x_2' = x_2, x_3' = -x_3$, and four additional elastic constants are found to be zero: $c_{1123} = c_{14}, c_{2223} = c_{24}, c_{3323} = c_{34}, c_{1312} = c_{56}$.

No additional information is obtained by rotating by π about $[001]$. Rotating by $2\pi/3$ anti-clockwise about $[111]$ results in $x_1' \to x_2, x_2' \to x_3, x_3' \to x_1$. Therefore the following elastic constants must be equal: $c_{1111} = c_{2222} = c_{3333}$; $c_{1122} = c_{2233} = c_{3311}$; $c_{2323} = c_{3131} = c_{1212}$, which in matrix notation are $c_{11} = c_{22} = c_{33}$; $c_{12} = c_{23} = c_{31}$; $c_{44} = c_{55} = c_{66}$. No additional information is obtained by invoking any of the other symmetry operations.

The conclusion is that there are three independent elastic constants in a cubic crystal: c_{11}, c_{12}, c_{44}:

$$\mathbf{c} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix}. \tag{3.21}$$

This conclusion remains the same with the cubic point group '432' in Hermann-Mauguin notation or O in Schönflies notation. Therefore, all cubic point groups have an elastic constant matrix of the same form as that shown in eqn.(3.21). This is neatly summarised in the following formula for the elastic constants in cubic crystals:

$$c_{ijkl} = c_{12}\delta_{ij}\delta_{kl} + c_{44}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + (c_{11} - c_{12} - 2c_{44})\,\delta_{ijkl} \tag{3.22}$$

where $\delta_{ijkl} = 1$ if $i = j = k = l$, zero otherwise.

The elements of the elastic constant matrix with value zero in a cubic crystal are the same as those in an isotropic medium. The only difference between the cubic and isotropic cases is that the anisotropy ratio, eqn.(3.13), in a cubic crystal is not unity. Let us look at this more closely. A pure shear strain e_{12} in a cubic crystal is on (100) and (010) planes, and it is created by the shear stress $\sigma_{12} = 2c_{44}e_{12}$. Therefore, c_{44} measure the resistance to shear on $\{100\}$ planes in the cubic crystal. If we rotate the coordinate system by $\pi/4$ about $[001]$ then e'_{12} is a pure shear on (110) and $(1\bar{1}0)$ planes. After transforming the elastic constant tensor it is found that $\sigma'_{12} = ((c_{11} - c_{12})/2)\,e'_{12}$. Therefore, $(c_{11} - c_{12})/2$ measures the resistance to shear on $\{110\}$ planes in the cubic crystal, and it is called C' (pronounced "C prime"). It follows that the anisotropy ratio in a cubic crystal is the ratio of the shear resistance on $\{100\}$ planes to the shear resistance on $\{110\}$ planes. In an isotropic crystal the resistances are the same. The anisotropy ratio can have a strong influence on the elastic fields of defects and modes of plastic deformation in cubic crystals.

3.5.2 The directional dependence of the elastic constants in anisotropic media

In an anisotropic medium the elastic constants vary with direction. For a chosen elastic constant this variation can be depicted graphically by plotting a surface $r(\theta, \phi)$ where r is the magnitude of the elastic constant along the direction (θ, ϕ) in spherical coordinates. In an isotropic medium this surface is a sphere.

As a first example consider the variation of c_{11} with direction in a cubic crystal. Orienting the Cartesian axes along the $\langle 100 \rangle$ directions as usual the variation of $c_{11} = c_{1111}$ as the coordinate system is rotated is given by eqn.(3.8):

$$c'_{1111} = R_{1i}R_{1j}R_{1k}R_{1l}c_{ijkl}. \tag{3.23}$$

Let $R_{1i} = \hat{\eta}_i$. This vector is parallel to the x'_1 axis. Equation (3.23) provides the value of c_{11} along the direction $\hat{\boldsymbol{\eta}}$ with respect to the cube axes. We obtain:

$$c'_{11} = c'_{1111} = c_{11} + 2(c_{11} - c_{12})\left(\frac{2c_{44}}{c_{11} - c_{12}} - 1\right)\left(\hat{\eta}_1^2\hat{\eta}_2^2 + \hat{\eta}_2^2\hat{\eta}_3^2 + \hat{\eta}_3^2\hat{\eta}_1^2\right), \tag{3.24}$$

where we see that the directional dependence is proportional to the deviation of the anisotropy ratio A (eqn.(3.13)) from unity. For $A > 1$ the maximum value of c'_{11} is along $\langle 111 \rangle$ directions. A plot of

c'_{11} is shown in Fig.3.1 for copper, where $c_{11} = 168.4$ GPa, $c_{12} = 121.4$ GPa, $c_{44} = 75.4$ GPa and the anisotropy ratio is $A = 3.21$. The average value of c'_{11}, where the averaging is over all directions, is $c_{11} + \frac{2}{5}(A-1)(c_{11} - c_{12})$, and in copper this is 210 GPa.

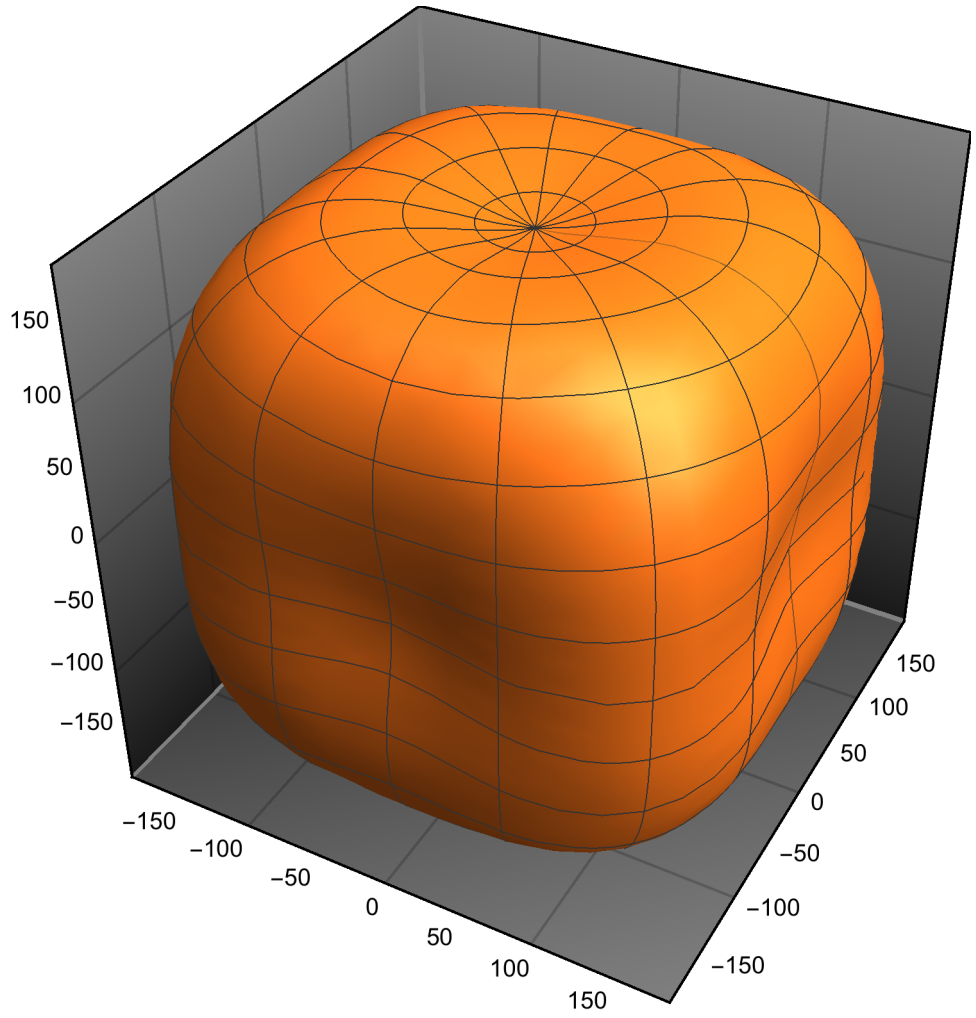

Figure 3.1: Polar plot of c'_{11} given by eqn.3.24 for copper. The axes are aligned with the $\langle 100 \rangle$ directions.

The variation of the shear elastic constant c_{44} with direction is more complicated because it depends on two directions: the plane normal and the direction of shear. Invoking the transformation law:

$$c'_{1212} = R_{1i}R_{2j}R_{1k}R_{2l}c_{ijkl} = \hat{\eta}_i\hat{\xi}_j\hat{\eta}_k\hat{\xi}_l c_{ijkl} \tag{3.25}$$

where $\hat{\xi}_j = R_{2j}$ is any unit vector perpendicular to $\hat{\boldsymbol{\eta}}$. In this equation $\hat{\boldsymbol{\eta}}$ may be interpreted as the normal to the plane where c'_{1212} is evaluated and $\hat{\boldsymbol{\xi}}$ as the direction of shear in that plane. Thus, c'_{1212} is a function of 3 independent variables. After some algebraic manipulations we obtain:

$$c'_{44} = c'_{66} = c'_{1212} = c_{44} - (c_{11} - c_{12})\left(\frac{2c_{44}}{c_{11} - c_{12}} - 1\right)\left(\hat{\eta}_1^2\hat{\xi}_1^2 + \hat{\eta}_2^2\hat{\xi}_2^2 + \hat{\eta}_3^2\hat{\xi}_3^2\right). \tag{3.26}$$

For example, when $\hat{\boldsymbol{\eta}} = [110]/\sqrt{2}$ and $\hat{\boldsymbol{\xi}} = [1\bar{1}0]/\sqrt{2}$ we obtain $c'_{44} = \frac{1}{2}(c_{11} - c_{12})$, which is C'. For completeness we also state the variation of the elastic constant c_{12} with two orthonormal directions $\hat{\boldsymbol{\eta}}$ and $\hat{\boldsymbol{\xi}}$:

$$c'_{12} = c'_{1122} = c_{12} - (c_{11} - c_{12})\left(\frac{2c_{44}}{c_{11} - c_{12}} - 1\right)\left(\hat{\eta}_1^2\hat{\xi}_1^2 + \hat{\eta}_2^2\hat{\xi}_2^2 + \hat{\eta}_3^2\hat{\xi}_3^2\right). \tag{3.27}$$

3.6 Further restrictions on the elastic constants

For structural stability the elastic energy density must be positive definite. Otherwise the material will spontaneously distort to a lower energy structure. The elastic energy density may be written in matrix notation as $\frac{1}{2}\sigma_i e_i = \frac{1}{2}c_{ij}e_i e_j$. For the quadratic form $c_{ij}e_i e_j$ to be positive definite all 6 of the leading principal minors of the 6×6 matrix $\mathbf{c}$ must be positive definite.

In an isotropic medium this condition leads to $\lambda + \frac{2}{3}\mu > 0$ and $\mu > 0$. Since the bulk modulus is given by $B = \lambda + \frac{2}{3}\mu$ (see eqn.(3.20)) the first condition is equivalent to requiring the bulk modulus is positive. In Exercise 3.6 it was also shown that the elastic energy density is positive definite provided $B > 0$ and $\mu > 0$.

In a cubic crystal the elastic energy density is positive definite provided $c_{11} - c_{12} > 0$, $c_{44} > 0$ and $c_{11} + 2c_{12} > 0$. Thus, the elastic energy density is positive definite provided the two shear elastic constants and the bulk modulus are all positive. c_{12} has to lie between $-c_{11}/2$ and c_{11}, and therefore Poisson's ratio, which is $c_{12}/(c_{11} + c_{12})$, has to lie between -1 and $\frac{1}{2}$.

3.7 Elastic constants and atomic interactions

Elastic constants may be calculated for a crystal if we have a description of atomic interactions. Consider a crystal with one atom at each lattice site. Since all atoms are at centres of inversion there is no net force acting on any atom. Let $u_i^{(n)}$ be a small arbitrary displacement of atom n. Then the change in the energy of the crystal to second order in the displacements is:

$$E = \sum_n \frac{\partial E}{\partial u_i^{(n)}} u_i^{(n)} + \frac{1}{2} \cdot \sum_n \sum_p \frac{\partial^2 E}{\partial u_i^{(n)} \partial u_j^{(p)}} u_i^{(n)} u_j^{(p)} \tag{3.28}$$

This is the usual harmonic expansion of the energy of the crystal, where the derivatives are evaluated in the perfect crystal configuration. The first term on the right is zero because the forces on all atoms are zero at equilibrium.

If $u_i^{(n)} = t_i$ for all n, where t_i is a small constant vector, then the energy E in eqn.(3.28) should be invariant, because the crystal has undergone a rigid body translation. This is achieved if the following equation is satisfied:

$$\frac{\partial^2 E}{\partial u_i^{(n)} \partial u_j^{(n)}} = -\sum_{p \neq n} \frac{\partial^2 E}{\partial u_i^{(n)} \partial u_j^{(p)}},$$

for each site n. When this is substituted into eqn.(3.28) the second order term becomes:

$$\begin{aligned} &\frac{1}{2} \cdot \sum_n \sum_p \frac{\partial^2 E}{\partial u_i^{(n)} \partial u_j^{(p)}} u_i^{(n)} u_j^{(p)} = \frac{1}{2} \cdot \sum_n \sum_{p \neq n} \frac{\partial^2 E}{\partial u_i^{(n)} \partial u_j^{(p)}} u_i^{(n)} (u_j^{(p)} - u_j^{(n)}) \\ = \quad &-\frac{1}{2} \cdot \frac{1}{2} \cdot \sum_n \sum_{p \neq n} \frac{\partial^2 E}{\partial u_i^{(n)} \partial u_j^{(p)}} (u_i^{(p)} - u_i^{(n)})(u_j^{(p)} - u_j^{(n)}) \end{aligned} \tag{3.29}$$

Let the displacements be created by a small homogeneous strain e_{kl}, such that $u_i^{(p)} - u_i^{(n)} = e_{ik}\left(X_k^{(p)} - X_k^{(n)}\right)$, where $\mathbf{X}^{(p)}$ is the position of atom p in the unstrained crystal. All atoms remain at centres of inversion during this operation and therefore the net force on any atom remains zero. Since the strain is homogeneous and since all atoms in the crystal remain equivalent we need to consider the change in the energy of just atom n, which we call δE_n:

$$\delta E_n = -\frac{1}{4}\sum_{p\neq n} e_{ik}\left(X_k^{(p)} - X_k^{(n)}\right) S_{ij}^{(np)} e_{jl}\left(X_l^{(p)} - X_l^{(n)}\right), \tag{3.30}$$

where $S_{ij}^{(np)} = \partial^2 E/\partial u_i^{(n)} \partial u_j^{(p)}$. We may rewrite this equation in terms of the elastic constants:

$$\delta E_n = \frac{1}{2}\Omega c_{ikjl}\, e_{ik}\, e_{jl}$$

where Ω is the volume of a primitive unit cell of the crystal. Comparing this with eqn.(3.30) we obtain:

$$c_{ikjl} = -\frac{1}{2\Omega}\sum_{p\neq n}\left(X_k^{(p)} - X_k^{(n)}\right) S_{ij}^{(np)}\left(X_l^{(p)} - X_l^{(n)}\right). \tag{3.31}$$

It is evident that this expression satisfies the symmetry $c_{ikjl} = c_{jlik}$. To satisfy the other symmetries of equations 3.6 we set $c_{ikjl} = \frac{1}{4}\left(c_{ikjl} + c_{kijl} + c_{iklj} + c_{kilj}\right)$:

$$\begin{aligned} c_{ikjl} = -\frac{1}{8\Omega}\Bigg\{ &\sum_{p\neq n}\left(X_k^{(p)} - X_k^{(n)}\right) S_{ij}^{(np)}\left(X_l^{(p)} - X_l^{(n)}\right) + \sum_{p\neq n}\left(X_i^{(p)} - X_i^{(n)}\right) S_{kj}^{(np)}\left(X_l^{(p)} - X_l^{(n)}\right) \\ &+ \sum_{p\neq n}\left(X_k^{(p)} - X_k^{(n)}\right) S_{il}^{(np)}\left(X_j^{(p)} - X_j^{(n)}\right) + \sum_{p\neq n}\left(X_i^{(p)} - X_i^{(n)}\right) S_{kl}^{(np)}\left(X_j^{(p)} - X_j^{(n)}\right)\Bigg\}. \end{aligned}$$

If there is more than one atom associated with each lattice site those atoms not on lattice sites may undergo small displacements in addition to those prescribed by a homogeneous strain. These additional displacements are sometimes called the 'internal strain'. Although the strain is still imposed by displacing atoms at lattice sites, atoms between lattice sites will experience net forces as a result of the strain if they are not at centres of inversion. Relaxation of those forces reduces the energy of the homogeneously strained crystal, and therefore it affects the calculated elastic constants.

3.8 Problem Set 3

1. In a face-centred cubic crystal with lattice constant a the 12 nearest neighbours of an atom are at $\pm a/2[110], \pm a/2[1\bar{1}0], \pm a/2[101], \pm a/2[10\bar{1}], \pm a/2[011], \pm a/2[01\bar{1}]$. Consider a model of the crystal in which the bonding is represented by linear springs, with spring constant k, between nearest neighbours only. By considering the elastic energy density of the crystal when an arbitrary small elastic strain is applied calculate the elastic constants c_{11}, c_{12} and c_{44}.
   Answers[6]: $c_{11} = 2k/a$ and $c_{12} = c_{44} = k/a$. It is interesting to note that the anisotropy ratio for this simple model is 2 and Poisson's ratio is $\frac{1}{3}$.

[6]The equality of c_{12} and c_{44} is a feature of all pairwise interaction models of cubic crystals. In these models it is assumed the energy is a sum of interactions between atoms taken in pairs. The energy of interaction between two atoms is

2. The Finnis-Sinclair model captures the dependence of the strength of the metallic bond between two atoms on the local atomic environment. This is a key feature of metallic bonding, and it is absent in models where the energy is a sum of pair potentials only. In the Finnis-Sinclair model the energy of the system is written as follows:

$$E = \left\{ \frac{1}{2} \sum_n \sum_{p \neq n} V\left(\left| \mathbf{X}^{(n)} - \mathbf{X}^{(p)} \right| \right) \right\} - \left\{ \sum_n \sqrt{ \sum_{p \neq n} \phi\left(\left| \mathbf{X}^{(n)} - \mathbf{X}^{(p)} \right| \right) } \right\} \tag{3.32}$$

   The first term on the right is a sum of pair potentials $V(r)$. Inside the square root of the second term is another sum of pair potentials $\phi(r)$. The square root may be justified using tight binding theory of electronic structure[7]. Show that this model does *not* satisfy the Cauchy relation $c_{12} = c_{44}$ in a cubic crystal.
3. Prove that c_{ijij} and c_{iijj} are invariants of the elastic constant tensor with respect to arbitrary rotations of the coordinate system.
4. Show that $c_{ijij} = c_{11} + c_{22} + c_{33} + 2(c_{44} + c_{55} + c_{66})$ and $c_{iijj} = c_{11} + c_{22} + c_{33} + 2(c_{12} + c_{13} + c_{23})$. Show that c_{iijj} is directly related to the bulk modulus in any crystal structure.
5. In a monoclinic crystal the only rotational symmetry is a two-fold rotation axis along x_3. Prove that the following elastic 8 constants are zero: $c_{14}, c_{15}, c_{24}, c_{25}, c_{34}, c_{35}, c_{46}, c_{56}$.
6. In an orthorhombic crystal there are two-fold rotation axes along each of the Cartesian axes x_1, x_2, x_3. Starting from the reduced elastic constant matrix of the monoclinic crystal prove that the effect of the two-fold rotation axes along x_1 or x_2 is to make the following 4 additional elastic constants zero: $c_{16}, c_{26}, c_{36}, c_{45}$. Hence show there are 9 independent elastic constants in an orthorhombic crystal.
7. In a tetragonal crystal the x_3-axis is a four-fold rotational symmetry axis. Starting from the reduced elastic constant matrix of the orthorhombic crystal prove that the effect of the four-fold rotation axis is to make: $c_{11} = c_{22}; c_{13} = c_{23}; c_{44} = c_{55}$. Hence show that there are 6 independent elastic constants in a tetragonal crystal with point group 422 (D_4): $c_{11}, c_{12}, c_{13}, c_{33}, c_{44}, c_{66}$. The only difference between this elastic constant matrix and the elastic constant matrix for hexagonal crystals is that c_{66} is no longer independent in a hexagonal crystal: $c_{66} = \frac{1}{2}(c_{11} - c_{12})$.
8. Show that in hexagonal crystals the elastic constant matrix is invariant with respect to rotations about the x_3 axis. The elastic constant matrix in a hexagonal crystal is as follows:

$$\mathbf{c} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(c_{11} - c_{12}) \end{bmatrix} \tag{3.33}$$

   This is why hexagonal crystals are described as 'transversely isotropic'.

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also assumed to depend only on their separation. In this question the pairwise interaction is the linear spring connecting a pair of neighbouring atoms. The experimental fact that c_{12} and c_{44} are not equal to each other in cubic crystals indicates that the pairwise interaction model fails as a description of atomic interactions. Not knowing any better in the 19th century Cauchy assumed a pairwise interaction model for all atomic interactions and showed there are six such relations between the elastic constants. They are: $c_{23} = c_{44}$; $c_{14} = c_{56}$; $c_{31} = c_{55}$; $c_{25} = c_{46}$; $c_{12} = c_{66}$; $c_{45} = c_{36}$. In a cubic crystal $c_{23} = c_{31} = c_{12}$ and $c_{66} = c_{55} = c_{44}$ so we expect c_{12} to equal c_{44}. These six equalities are known as the Cauchy relations and Cauchy used them to argue (incorrectly) that the maximum number of independent elastic constants is not 21 but 15. The Cauchy relations are now only of historical significance.

[7] see *Electronic structure of materials*, A. P. Sutton (1993), p. 179-182

9. Show that the following restrictions must apply to the elastic constants in a hexagonal crystal: $c_{11} > 0$; $c_{11} > c_{12}$; $c_{44} > 0$; $c_{33}(c_{11} + c_{12}) > 2c_{13}^2$.
10. If the elastic constants of a crystal are averaged over all possible orientations with respect to a fixed coordinate system the elastic constants obtained are those of an isotropic medium. To obtain the elastic constants λ and μ of this isotropic medium we can use the two invariants of the elastic constant tensor c_{ijij} and c_{iijj} mentioned in problem 4.

    Show that in an isotropic medium $c_{ijij} = 3\lambda + 12\mu$ and $c_{iijj} = 9\lambda + 6\mu$.

    In a cubic crystal show that $c_{ijij} = 3c_{11} + 6c_{44}$ and $c_{iijj} = 3c_{11} + 6c_{12}$.

    Hence show that:

$$\begin{aligned} \lambda &= c_{12} + \frac{1}{5}(c_{11} - c_{12} - 2c_{44}) \\ \mu &= c_{44} + \frac{1}{5}(c_{11} - c_{12} - 2c_{44}) \end{aligned}$$

    Hence show that the average values of c_{11}, c_{12} and c_{44} over all orientations of a cubic crystal are given by:

$$\begin{aligned} 5\langle c_{11}\rangle &= 3c_{11} + 2c_{12} + 4c_{44} \\ 5\langle c_{12}\rangle &= c_{11} + 4c_{12} - 2c_{44} \\ 5\langle c_{44}\rangle &= c_{11} - c_{12} + 3c_{44} \end{aligned} \tag{3.34}$$

    where $\langle c_{11}\rangle = \langle c_{12}\rangle + 2\langle c_{44}\rangle$. These averages may be obtained directly from eqns.(3.24, 3.27 and 3.26) respectively.

4. The elastic Green's function

4.1 Differential equation for the displacement field

Imagine you are applying pressure with your finger against a piece of supported rubber. You see the rubber distorts until you can't push any further. Equilibrium has been achieved between the force you are applying through your finger and the stresses created within the rubber by the distortion. This is the physics of eqn.(2.15): $\sigma_{ij,j}(\mathbf{x}) + f_i(\mathbf{x}) = 0$. The force f_i acting at $\mathbf{x}$ creates a stress field with a divergence that exactly balances the force and keeps the body in equilibrium. We can make this more explicit by using the divergence theorem. Let the body force be a point force located at $\mathbf{x}_0$, such that $f_i(\mathbf{x}) = \mathscr{F}_i \delta(\mathbf{x} - \mathbf{x}_0)$. Then we can write:

$$\int_{\mathscr{R}} f_i \, \mathrm{d}V = \int_{\mathscr{R}} \mathscr{F}_i \delta(\mathbf{x} - \mathbf{x}_0) \, \mathrm{d}V = \mathscr{F}_i = -\int_{\mathscr{R}} \sigma_{ij,j} \, \mathrm{d}V = -\int_{\mathscr{S}} \sigma_{ij} n_j \, \mathrm{d}S. \tag{4.1}$$

Here $\mathscr{R}$ is any region in the continuum containing the body force at $\mathbf{x}_0$. The surface of $\mathscr{R}$ is $\mathscr{S}$. The stresses created by the distortion of the medium in response to the body force at $\mathbf{x}_0$ give rise to tractions, $\sigma_{ij} n_j$, on the surface $\mathscr{S}$, which when integrated over the whole surface surrounding $\mathscr{R}$ exactly cancel the force $\mathscr{F}_i$.

If we substitute Hooke's law into the equilibrium condition $\sigma_{ij,j}(\mathbf{x}) + f_i(\mathbf{x}) = 0$ we obtain a differential equation for the strain field created by the body force: $c_{ijkl} \, e_{kl,j}(\mathbf{x}) + f_i(\mathbf{x}) = 0$. If we then use the relationship between the strain and the displacement field, $e_{kl}(\mathbf{x}) = \frac{1}{2}(u_{k,l}(\mathbf{x}) + u_{l,k}(\mathbf{x}))$ we obtain a second order differential equation for the displacement field:

$$c_{ijkl} \, u_{k,lj}(\mathbf{x}) + f_i(\mathbf{x}) = 0, \tag{4.2}$$

where we have used the symmetry of the elastic constant tensor to write $c_{ijkl} \, u_{l,k} = c_{ijlk} \, u_{l,k}$, and then we equated $c_{ijlk} \, u_{l,k}$ to $c_{ijkl} \, u_{k,l}$. The assertion that the strain field is the symmetrized gradient of the displacement field, $e_{kl}(\mathbf{x}) = \frac{1}{2}(u_{k,l}(\mathbf{x}) + u_{l,k}(\mathbf{x}))$, ensures that the material surrounding the

region of the body force fits together compatibly, that is with no holes or overlapping material[1]. This assertion cannot be made where the body forces act.

Equation 4.2 plays the same role in elasticity as Poisson's equation in electrostatics. The equivalent in elasticity of Laplace's equation in electrostatics is $c_{ijkl}\,u_{k,lj} = 0$. Whereas electrostatics relies on invisible electric fields and 'action at a distance' to transmit forces between charges, in elasticity the forces acting between defects in the material are conveyed by the elastic displacement field which is real and can sometimes be seen in detail in the electron microscope using modern imaging techniques.

The apparent simplicity of eqn.(4.2) is deceptive. It comprises three equations, one for each component of the body force. Each of these equations involves second derivatives of all three components of the displacement field. Below we consider the simplest case, which arises when the isotropic elastic approximation is made.

Boundary value problems in elasticity amount to finding solutions of eqn.(4.2) subject to boundary conditions of three principal types. The first is where displacements are prescribed on the surface of the body. The second is where tractions on the surface of the body are prescribed. The third is a mixture of the first two, where displacements are prescribed on parts of the surface of the body and tractions on the surface of the body where displacements are not prescribed. There are uniqueness theorems for the solutions of eqn.(4.2) for both simply connected and multiply connected bodies[2].

4.1.1 Navier's equation

The elastic constant tensor in isotropic elasticity is conveniently expressed in eqn.(3.11). When this is inserted into eqn.(4.2) we obtain the following differential equation:

$$\mu u_{i,jj} + (\lambda + \mu) u_{k,ki} + f_i = 0, \tag{4.3}$$

which can be expressed in vector form as follows:

$$\mu \nabla^2 \mathbf{u} + (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}) + \mathbf{f} = 0. \tag{4.4}$$

This is known as Navier's equation[3].

Exercise 4.1 Derive eqn.(4.3) from eqn.(3.11) and eqn.(4.2). ∎

4.2 The physical meaning of the elastic Green's function and why it is useful

4.2.1 Definition of the elastic Green's function

We consider an infinite homogeneous elastic medium in which there is a point force $\mathbf{f}$ acting at $\mathbf{x} = \mathbf{x}_0$. The elastic Green's function gives the elastic displacement field created by this point force:

$$u_i(\mathbf{x}) = G_{ij}(\mathbf{x} - \mathbf{x}_0)\, f_j(\mathbf{x}_0). \tag{4.5}$$

[1] For an illuminating discussion of compatibility and incompatibility see section 10 of *Micromechanics of defects in solids* by T. Mura, 2nd ed. (1987) Kluwer: Dordrecht.

[2] see section 6.2 of *Elastic models of crystal defects*, C. Teodosiu Springer Velag: Berlin (1982)

[3] Claude-Louis Navier (1785-1836)

This may be taken as the definition of the elastic Green's function, although it does not by itself enable the Green's function to be evaluated. Since eqn.(4.2) is linear the displacement due to a distribution of body forces $\mathbf{f}(\mathbf{x})$ is found by linear superposition:

$$u_i(\mathbf{x}) = \int G_{ij}(\mathbf{x}-\mathbf{x}')\, f_j(\mathbf{x}')\mathrm{d}^3x'. \tag{4.6}$$

The elastic fields of all structural defects in crystals arise from forces on atoms in the centre of the defect, otherwise known as the core of the defect. Those atoms move from their perfect crystal positions until the forces on them are counteracted by forces from their neighbours, including those further from the defect. The neighbours of the neighbours move from their ideal crystal positions until the net forces on them return to zero, and so the displacement field spreads from the defect. The displacements each neighbour shell undergoes decays with distance from the defect because the forces are distributed among more atoms. For example, consider a missing atom in a crystal, which is called a vacancy. The atoms neighbouring the vacancy experience a net force as a result of the missing atom. They move in response to the net forces acting on them, which sets up forces on their neighbours, and so their neighbours also move but by generally smaller amounts. When equilibrium is re-established the net force acting on any atom is zero and an elastic displacement field is set up in the crystal which decays, in an infinite crystal, as the inverse square of the distance from the vacancy.

The elastic Green's function is unlikely to estimate accurately the displacements of atoms in the core of the defect where the forces may be very large. In this region it is best to use an atomistic model with a sound description of atomic interactions. But it is generally found that at distances of no more than a nanometre from the defect core the description of the relaxation displacements is quite accurately described by linear anisotropic elasticity. Conversely, atomistic models are inappropriate for long-range interactions between defects partly because the numbers of atoms involved may be far greater than can be treated computationally, but also because elasticity theory is likely to be more accurate and certainly more informative for long-range interactions.

Before we derive the equation that determines the elastic Green's function we note some of its properties. First, since the medium is assumed to be homogeneous it follows that G_{ij} depends only on the relative position of the field point $\mathbf{x}$ and the location $\mathbf{x}_0$ of the point force. If the material were inhomogeneous then G_{ij} would become a function of both $\mathbf{x}$ and $\mathbf{x}_0$. Secondly, $G_{ij}(\mathbf{x}) = G_{ij}(-\mathbf{x})$ because the infinite, homogeneous elastic continuum is everywhere centrosymmetric.

Thirdly, $G_{ij}(\mathbf{x}) = G_{ji}(\mathbf{x})$. This follows from a result in mechanics, known as Maxwell's reciprocity theorem[4]. Suppose we apply a point force $\mathbf{F}^{(1)}$ gradually at $\mathbf{x}^{(1)}$. It produces a displacement $\mathbf{u}^{(1)}$ at $\mathbf{x}^{(1)}$, and the work done is $W^{(1)} = \frac{1}{2}\mathbf{F}^{(1)} \cdot \mathbf{u}^{(1)}(\mathbf{x}^{(1)})$. The factor of $\frac{1}{2}$ is because the force is gradually built up from zero to $\mathbf{F}^{(1)}$, during which the displacement of $\mathbf{x}^{(1)}$ increases linearly from zero to $\mathbf{u}^{(1)}$. Now we introduce the force $\mathbf{F}^{(2)}$ gradually at $\mathbf{x}^{(2)}$. The additional work done is $W^{(2)} + W^{(12)}$ where $W^{(2)} = \frac{1}{2}\mathbf{F}^{(2)} \cdot \mathbf{u}^{(2)}(\mathbf{x}^{(2)})$ and $W^{(12)} = \mathbf{F}^{(1)} \cdot \mathbf{u}^{(2)}(\mathbf{x}^{(1)})$. Note the absence of the factor of $\frac{1}{2}$ in $W^{(12)}$ because the force $\mathbf{F}^{(1)}$ at $\mathbf{x}^{(1)}$ already exists in full. Thus the total work done is $\frac{1}{2}\mathbf{F}^{(1)} \cdot \mathbf{u}^{(1)}(\mathbf{x}^{(1)}) + \frac{1}{2}\mathbf{F}^{(2)} \cdot \mathbf{u}^{(2)}(\mathbf{x}^{(2)}) + \mathbf{F}^{(1)} \cdot \mathbf{u}^{(2)}(\mathbf{x}^{(1)})$. Now repeat the process, but introduce the force $\mathbf{F}^{(2)}$ gradually at $\mathbf{x}^{(2)}$ and then introduce the force $\mathbf{F}^{(1)}$ gradually at $\mathbf{x}^{(1)}$. The total work done must be same, but now it is $\frac{1}{2}\mathbf{F}^{(1)} \cdot \mathbf{u}^{(1)}(\mathbf{x}^{(1)}) + \frac{1}{2}\mathbf{F}^{(2)} \cdot \mathbf{u}^{(2)}(\mathbf{x}^{(2)}) + \mathbf{F}^{(2)} \cdot \mathbf{u}^{(1)}(\mathbf{x}^{(2)})$. Thus, we arrive at Maxwell's reciprocity relation:

$$\mathbf{F}^{(1)} \cdot \mathbf{u}^{(2)}(\mathbf{x}^{(1)}) = \mathbf{F}^{(2)} \cdot \mathbf{u}^{(1)}(\mathbf{x}^{(2)}) \tag{4.7}$$

[4]James Clerk Maxwell FRS (1831-1879). The theorem is in this paper: J. Clerk Maxwell F.R.S. (1864) L. *On the calculation of the equilibrium and stiffness of frames*, Philosophical Magazine, **27**, issue182, 294-299. Available online at `http://www.tandfonline.com/doi/abs/10.1080/14786446408643668`

This says that the work done by a force $\mathbf{F}^{(1)}$ when its point of application is displaced by $\mathbf{u}^{(2)}$ due to another force $\mathbf{F}^{(2)}$ is equal to the work done by the force $\mathbf{F}^{(2)}$ when its point of application is displaced by $\mathbf{u}^{(1)}$ due to the force $\mathbf{F}^{(1)}$. Since $u_i^{(1)}(\mathbf{x}^{(2)}) = G_{ij}(\mathbf{x}^{(2)} - \mathbf{x}^{(1)})F_j^{(1)}$ and $u_i^{(2)}(\mathbf{x}^{(1)}) = G_{ij}(\mathbf{x}^{(1)} - \mathbf{x}^{(2)})F_j^{(2)}$ then the left hand side of eqn.(4.7) becomes:

$$F_i^{(1)} u_i^{(2)}(\mathbf{x}^{(1)}) = F_i^{(1)} G_{ij}(\mathbf{x}^{(1)} - \mathbf{x}^{(2)}) F_j^{(2)}$$

and the right-hand side becomes

$$F_i^{(2)} u_i^{(1)}(\mathbf{x}^{(2)}) = F_i^{(2)} G_{ij}(\mathbf{x}^{(2)} - \mathbf{x}^{(1)}) F_j^{(1)} = F_j^{(2)} G_{ji}(\mathbf{x}^{(2)} - \mathbf{x}^{(1)}) F_i^{(1)} = F_i^{(1)} G_{ji}(\mathbf{x}^{(1)} - \mathbf{x}^{(2)}) F_j^{(2)},$$

where we have used $G_{ij}(\mathbf{x}) = G_{ij}(-\mathbf{x})$. Therefore, $G_{ij}(\mathbf{x}) = G_{ji}(\mathbf{x})$.

4.2.2 The equation for the elastic Green's function in an infinite medium

In this section we derive a partial differential equation for the elastic Green's function. Consider a point force $\mathbf{F}$ applied at $\mathbf{x}_0$ in an infinite, homogeneous elastic continuum. From the definition of the Green's function, eqn.(4.5), this force sets up an elastic displacement field given by $u_i(\mathbf{x}) = G_{ij}(\mathbf{x} - \mathbf{x}_0)F_j(\mathbf{x}_0)$. Differentiating this displacement field and using Hooke's law we find the stress field associated with this displacement field is as follows:

$$\sigma_{kp}(\mathbf{x}) = c_{kpim} G_{ij,m}(\mathbf{x} - \mathbf{x}_0) F_j(\mathbf{x}_0),$$

where the derivative of the Green's function is with respect to x_m. Consider any region $\mathscr{R}$, with surface $\mathscr{S}$, containing $\mathbf{x}_0$. For mechanical equilibrium we must have:

$$F_k(\mathbf{x}_0) + \int_{\mathscr{S}} \sigma_{kp}(\mathbf{x})\, n_p \, \mathrm{d}^2 x = 0,$$

where n_p is the outward normal at $\mathbf{x}$ to the surface $\mathscr{S}$. Therefore,

$$F_k(\mathbf{x}_0) + \int_{\mathscr{S}} c_{kpim} G_{ij,m}(\mathbf{x} - \mathbf{x}_0) F_j(\mathbf{x}_0)\, n_p \, \mathrm{d}^2 x = 0.$$

Applying the divergence theorem to the surface integral we transform it into a volume integral over $\mathscr{R}$:

$$F_k(\mathbf{x}_0) + \int_{\mathscr{R}} c_{kpim} G_{ij,mp}(\mathbf{x} - \mathbf{x}_0) F_j(\mathbf{x}_0)\, \mathrm{d}^3 x = 0.$$

We bring $F_k(\mathbf{x}_0)$ inside the volume integral by writing it as $\int_{\mathscr{R}} \delta_{jk}\, \delta(\mathbf{x} - \mathbf{x}_0) F_j(\mathbf{x}_0) \mathrm{d}^3 x$, where the integration is again over $\mathbf{x}$ inside the region $\mathscr{R}$. We then obtain:

$$\int_{\mathscr{R}} \left[c_{kpim} G_{ij,mp}(\mathbf{x} - \mathbf{x}_0) + \delta_{jk}\, \delta(\mathbf{x} - \mathbf{x}_0) \right] F_j(\mathbf{x}_0)\, \mathrm{d}^3 x = 0.$$

Since this must hold for all point forces at $\mathbf{x}_0$, and for all regions $\mathscr{R}$ containing $\mathbf{x}_0$, the expression in square brackets must be zero:

$$c_{kpim}G_{ij,mp}(\mathbf{x}-\mathbf{x}_0)+\delta_{jk}\,\delta(\mathbf{x}-\mathbf{x}_0)=0. \tag{4.8}$$

This is the partial differential equation that enables us to calculate the Green's function.

Exercise 4.2 Show that $\delta(h\mathbf{x})=(1/|h|^3)\delta(\mathbf{x})$, where h is any scaling factor. Therefore the delta function in eqn.(4.8) behaves as a homogeneous function of degree -3. Hence show that

$$G_{ij}(\mathbf{x}-\mathbf{x}_0)=\frac{1}{|\mathbf{x}-\mathbf{x}_0|}\,g_{ij}, \tag{4.9}$$

where g_{ij} depends only on the orientation of $\mathbf{x}-\mathbf{x}_0$. This separation of the Green's function into radial and orientational dependencies applies in all cases regardless of the degree of anisotropy. ■

4.2.3 Solving boundary value problems with the elastic Green's function

This section illustrates the usefulness of the Green's function for solving boundary value problems. To do this we do not need explicit functional forms for the Green's function, only its defining differential equation, eqn.(4.8). We will see how and why we can use the Green's function for an infinite medium even when we are dealing with a finite medium, which of course has a surface. We shall use two spatial variables $\mathbf{x}$ and $\mathbf{x}'$. Differentiation with respect to the primed variable will be indicated by a prime on the subscript, thus $\partial f/\partial x'_m \equiv f_{,m'}$. If there is no prime on a subscript after a comma it signifies differentiation with to the corresponding component of $\mathbf{x}$.

All linear elastic fields must satisfy the equation of mechanical equilibrium, eqn.(4.2):

$$c_{kpim}\,u_{i,m'p'}(\mathbf{x}')+f_k(\mathbf{x}')=0. \tag{4.10}$$

Replacing $\mathbf{x}_0$ in eqn.(4.8) with $\mathbf{x}'$ the Green's function $G_{ij}(\mathbf{x}-\mathbf{x}')$ satisfies:

$$c_{kpim}G_{ij,mp}(\mathbf{x}-\mathbf{x}')+\delta_{jk}\,\delta(\mathbf{x}-\mathbf{x}')=0. \tag{4.11}$$

Multiplying eqn.(4.11) by $u_k(\mathbf{x}')$ and eqn.(4.10) by $G_{kj}(\mathbf{x}-\mathbf{x}')$ and subtracting we obtain:

$$c_{kpim}G_{ij,mp}(\mathbf{x}-\mathbf{x}')u_k(\mathbf{x}')+\delta_{jk}\,\delta(\mathbf{x}-\mathbf{x}')u_k(\mathbf{x}')-c_{kpim}\,u_{i,m'p'}(\mathbf{x}')G_{kj}(\mathbf{x}-\mathbf{x}')-f_k(\mathbf{x}')G_{kj}(\mathbf{x}-\mathbf{x}')=0.$$

Integrating this equation with respect to $\mathbf{x}'$ over a region $\mathscr{R}$ containing $\mathbf{x}$ we get:

$$\begin{aligned} u_j(\mathbf{x}) &= \int_{\mathscr{R}} G_{jk}(\mathbf{x}-\mathbf{x}')f_k(\mathbf{x}')\mathrm{d}^3x' \\ &+ \int_{\mathscr{R}} c_{kpim}\,u_{i,m'p'}(\mathbf{x}')\,G_{kj}(\mathbf{x}-\mathbf{x}')\,\mathrm{d}^3x' \\ &- \int_{\mathscr{R}} c_{kpim}\,G_{ij,m'p'}(\mathbf{x}-\mathbf{x}')\,u_k(\mathbf{x}')\mathrm{d}^3x', \end{aligned}$$

where we have used $G_{ij,mp}(\mathbf{x}-\mathbf{x}') = G_{ij,m'p'}(\mathbf{x}-\mathbf{x}')$. We can combine the last two volume integrals as follows:

$$\int_{\mathscr{R}} c_{kpim}\, u_{i,m'p'}(\mathbf{x}')\, G_{kj}(\mathbf{x}-\mathbf{x}')\, \mathrm{d}^3x' - \int_{\mathscr{R}} c_{kpim}\, G_{ij,m'p'}(\mathbf{x}-\mathbf{x}')\, u_k(\mathbf{x}')\mathrm{d}^3x' =$$
$$\int_{\mathscr{R}} c_{kpim}\left[u_{i,m'}(\mathbf{x}')\, G_{kj}(\mathbf{x}-\mathbf{x}') - u_k(\mathbf{x}')G_{ij,m'}(\mathbf{x}-\mathbf{x}')\right]_{,p'},$$

where we have used the symmetry of the elastic constant tensor $c_{kpim} = c_{imkp}$ to achieve a cancellation of two additional terms that arise in the differentiation of the expression in square brackets. Applying the divergence theorem to the resulting volume integral we obtain the following surface integrals over the surface $\mathscr{S}$ of the region $\mathscr{R}$:

$$\int_{\mathscr{R}} c_{kpim}\left[u_{i,m'}(\mathbf{x}')\, G_{kj}(\mathbf{x}-\mathbf{x}') - u_k(\mathbf{x}')G_{ij,m'}(\mathbf{x}-\mathbf{x}')\right]_{,p'} =$$
$$\int_{\mathscr{S}} G_{jk}(\mathbf{x}-\mathbf{x}')\, c_{kpmi}\, u_{i,m'}(\mathbf{x}')\, n_{p'}\, \mathrm{d}^2x' - \int_{\mathscr{S}} G_{ji,m'}(\mathbf{x}-\mathbf{x}')\, c_{mikp}\, u_k(\mathbf{x}')\, n_{p'}\, \mathrm{d}^2x',$$

where we observe that $c_{kpmi}\, u_{i,m'}\, n_{p'} = \sigma_{kp}(\mathbf{x}')\, n_{p'} = t_k(\mathbf{x}')$ is the traction acting on $\mathscr{S}$ at $\mathbf{x}'$. Replacing the last two volume integrals in the above equation for $u_j(\mathbf{x})$ with these two surface integrals we obtain finally:

$$\begin{aligned} u_j(\mathbf{x}) &= \int_{\mathscr{R}} G_{jk}(\mathbf{x}-\mathbf{x}')\, f_k(\mathbf{x}')\, \mathrm{d}^3x' \\ &+ \int_{\mathscr{S}} G_{jk}(\mathbf{x}-\mathbf{x}')\, t_k(\mathbf{x}')\mathrm{d}^2x' \\ &- \int_{\mathscr{S}} G_{ji,m'}(\mathbf{x}-\mathbf{x}')\, c_{mikp}\, u_k(\mathbf{x}')\, n_{p'}\, \mathrm{d}^2x'. \end{aligned} \tag{4.12}$$

Here are some observations to illustrate the usefulness of this result. First, consider a distribution of body force, such as that created by a structural defect, inside a finite body with free surfaces. If we use only the first line of eqn.(4.12) to evaluate the displacement field in the finite body the answer will be wrong because the Green's function is constructed for an infinite body. In particular, this displacement field will predict tractions at the surface of the finite body, when the surface should be free of such tractions. To correct for this we may calculate the displacement field caused by an equal and opposite distribution of surface tractions using the second line of eqn.(4.12). We may then use the superposition principle and add this to the displacements caused by the distribution of body forces in the first line to obtain the correct solution with surfaces free of tractions. In this way we are able to use the Green's function for an infinite body to solve a problem in a finite body, which is very convenient because all bodies are finite in practice. Secondly, if there are additional tractions applied to the surface of the body they may be included in the surface integral on the second line. The surface integral on the third line is used when displacements are specified on the surface $\mathscr{S}$. Here the surface may include a cut made from the external surface of the body into some point inside the body, where there is a discontinuity in the displacement across the cut. This will be very useful when we discuss dislocations in Chapter 6.

It may be puzzling that the derivative of the Green's function appears in the third line of eqn.(4.12) to satisfy the boundary condition where a displacement is specified. To get some insight into this we offer a slightly modified version of an argument from the book[5] by Landau[6] and Lifshitz[7]. Consider an infinite planar fault with unit normal $\hat{\mathbf{n}}$ in an infinite continuum. The half space on the negative side of the fault has the displacement vector $\mathbf{u} = \boldsymbol{\tau}/2$, and $\mathbf{u} = -\boldsymbol{\tau}/2$ in the positive half space. To deal with the singularity in the displacement gradient in the plane of the fault we assign a finite thickness Δ to the fault, and subsequently take the limit that $\Delta \to 0$. The displacement gradient is then $u_{i,k} = -\tau_i n_k/\Delta$ inside the fault and zero outside. The strain tensor is the constant value $e_{ik} = -\frac{1}{2}(\tau_i n_k + n_i \tau_k)/\Delta$ inside the fault and zero outside. Thus the stress changes discontinuously at the planes where the faulted region begins and ends. Discontinuous changes in stress are unphysical because they correspond to infinite forces. Therefore we use the equilibrium condition $\sigma_{im,m} + f_i = 0$ to introduce sheets of body force to cancel these discontinuities. The displacement field is then given by:

$$\begin{aligned}
u_i(\mathbf{x}) &= \int_{\text{all space}} G_{ij}(\mathbf{x}-\mathbf{x}') f_j(\mathbf{x}') \mathrm{d}^3 x' \\
&= -\int_{\text{all space}} G_{ij}(\mathbf{x}-\mathbf{x}') \sigma_{jm,m'}(\mathbf{x}') \mathrm{d}^3 x' \\
&= -\int_{\text{all space}} G_{ij}(\mathbf{x}-\mathbf{x}') c_{jmkl} e_{kl,m'}(\mathbf{x}') \mathrm{d}^3 x' \\
&= -\int_{\text{all space}} \left\{ \left(G_{ij}(\mathbf{x}-\mathbf{x}') c_{jmkl} e_{kl}(\mathbf{x}') \right)_{,m'} - G_{ij,m'}(\mathbf{x}-\mathbf{x}') c_{jmkl} e_{kl}(\mathbf{x}') \right\} \mathrm{d}^3 x' \\
&= -\int_{\text{fault surfaces}} \left(G_{ij}(\mathbf{x}-\mathbf{x}') c_{jmkl} e_{kl}(\mathbf{x}') \right) n_{m'} \mathrm{d}^2 x' + \int_{\text{all space}} G_{ij,m'}(\mathbf{x}-\mathbf{x}') c_{jmkl} e_{kl}(\mathbf{x}') \mathrm{d}^3 x'.
\end{aligned}$$

The surface integral is over the surfaces of the fault region where the displacement gradient begins and ends. In the limit $\Delta \to 0$ these integrals cancel because the surface normal changes sign on either side of the fault. The region of integration in the volume integral in the last line reduces to the volume occupied by the fault, which is Δ per unit area; this cancels the Δ in the denominator of e_{kl}. As $\Delta \to 0$ we obtain:

$$\begin{aligned}
u_i(\mathbf{x}) &= -\int_{\text{fault plane}} G_{ij,m'}(\mathbf{x}-\mathbf{x}') c_{jmkl} \frac{1}{2}(\tau_k n_l + n_k \tau_l) \mathrm{d}^2 x' \\
&= -\int_{\text{fault plane}} G_{ij,m'}(\mathbf{x}-\mathbf{x}') c_{jmkl} \tau_k n_l \mathrm{d}^2 x', \qquad (4.13)
\end{aligned}$$

where we have used the symmetry of the elastic constant tensor $c_{jmkl} = c_{jmlk}$ in the final integral.

In summary, to create a fault with normal $\hat{\mathbf{n}}$ and a constant relative translation of $\boldsymbol{\tau}$ we introduce dipolar sheets of forces in planes on either side of the fault. It is because the constant displacement is created by force dipoles that the derivative of the Green's function is involved. There is an analogy here between a shift in the electrostatic potential across an interface and the presence of a layer of charge dipoles at the interface.

[5] L. D Landau and E. M. Lifshitz, *Theory of Elasticity*, Pergamon Press: Oxford, 3rd edition (1986), section 27, p.111

[6] Lev Davidovich Landau (1908-1968) Nobel prize winning Soviet physicist

[7] Evgeny Mikhailovich Lifshitz ForMemRS (1915-1985) Soviet physicist

4.3 A general formula for the elastic Green's function in anisotropic media

We turn now to deriving a general formula for the elastic Green's function in an anisotropic continuum. We shall follow the treatment given in the review[8] by Bacon, Barnett and Scattergood. There are only two cases where the Green's function can be obtained in closed form analytically, and they are the cases of elastic isotropy and hexagonal symmetry.

We start from eqn.(4.8):

$$c_{jlms} G_{mp,ls}(\mathbf{x}) + \delta_{jp}\,\delta(\mathbf{x}) = 0,$$

where we have used the translational invariance of the infinite, homogeneous continuum to replace $\mathbf{x} - \mathbf{x}_0$ with just $\mathbf{x}$. Taking the Fourier transform of this equation we obtain:

$$c_{jlms} k_l k_s \tilde{G}_{mp}(\mathbf{k}) = \delta_{jp},$$

where

$$\begin{aligned} \tilde{G}_{mp}(\mathbf{k}) &= \int G_{mp}(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3 x \\ G_{mp}(\mathbf{x}) &= \frac{1}{(2\pi)^3} \int \tilde{G}_{mp}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3 k. \end{aligned}$$

We now introduce a matrix (kk) that plays a central role in many aspects of anisotropic elasticity. It is where all the information about the elastic constants is held:

$$(kk)_{jm} = c_{jlms} k_l k_s, \tag{4.14}$$

Note that (kk) is a symmetric matrix. The 3×3 matrix of Fourier transforms is just the inverse of the matrix (kk):

$$\tilde{G}_{mp}(\mathbf{k}) = \left[(kk)^{-1}\right]_{mp},$$

where we put square brackets around $(kk)^{-1}$ to make clear that $\tilde{G}_{mp}(\mathbf{k})$ is the mp-element of the inverse matrix of (kk) not the inverse of the matrix element $(kk)_{mp}$. Taking the inverse transform we obtain:

$$G_{mp}(\mathbf{x}) = \frac{1}{(2\pi)^3} \int \left[(kk)^{-1}\right]_{mp} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3 k \tag{4.15}$$

We introduce some additional vectors to help us evaluate this triple integral. Let the unit vectors $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3$ be aligned with the Cartesian axes used to define the elastic constant tensor. We may express $\mathbf{x}$ in spherical polar coordinates defined with respect to $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3$ as follows:

$$\mathbf{x} = x\,\hat{\boldsymbol{\rho}} = x\left[\sin\theta\cos\phi\,\hat{\mathbf{e}}_1 + \sin\theta\sin\phi\,\hat{\mathbf{e}}_2 + \cos\theta\,\hat{\mathbf{e}}_3\right],$$

where we have also introduced x as the length of $\mathbf{x}$ and $\hat{\boldsymbol{\rho}}$ as the direction of $\mathbf{x}$. It is useful to introduce two more orthonormal vectors $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ which are perpendicular to $\mathbf{x}$, such that $\hat{\mathbf{a}}, \hat{\mathbf{b}}$ and $\hat{\boldsymbol{\rho}}$ form a right-handed set, $\hat{\mathbf{a}} \times \hat{\mathbf{b}} = \hat{\boldsymbol{\rho}}$:

[8] D J Bacon, D M Barnett and R O Scattergood, *Anisotropic continuum theory of lattice defects*, Progress in Materials Science, **23**, 51-262 (1979). Available online at `https://doi.org/10.1016/0079-6425(80)90007-9`

$$\begin{aligned}\hat{\mathbf{a}} &= \sin\phi\hat{\mathbf{e}}_1 - \cos\phi\hat{\mathbf{e}}_2 \\ \hat{\mathbf{b}} &= \cos\theta\cos\phi\hat{\mathbf{e}}_1 + \cos\theta\sin\phi\hat{\mathbf{e}}_2 - \sin\theta\hat{\mathbf{e}}_3 \\ \hat{\boldsymbol{\rho}} &= \sin\theta\cos\phi\hat{\mathbf{e}}_1 + \sin\theta\sin\phi\hat{\mathbf{e}}_2 + \cos\theta\hat{\mathbf{e}}_3.\end{aligned}$$

Let k be the length of the vector $\mathbf{k}$ and let $\hat{\boldsymbol{\xi}}$ be the direction of $\mathbf{k}$. Then $\mathbf{k}$ may be expressed in the coordinate system $\hat{\mathbf{a}}, \hat{\mathbf{b}}, \hat{\boldsymbol{\rho}}$ as follows:

$$\mathbf{k} = k\hat{\boldsymbol{\xi}} = k\left[\sin\zeta\cos\psi\hat{\mathbf{a}} + \sin\zeta\sin\psi\hat{\mathbf{b}} + \cos\zeta\hat{\boldsymbol{\rho}}\right],$$

where ζ is the angle between $\mathbf{x}$ and $\mathbf{k}$, see Fig.4.1.

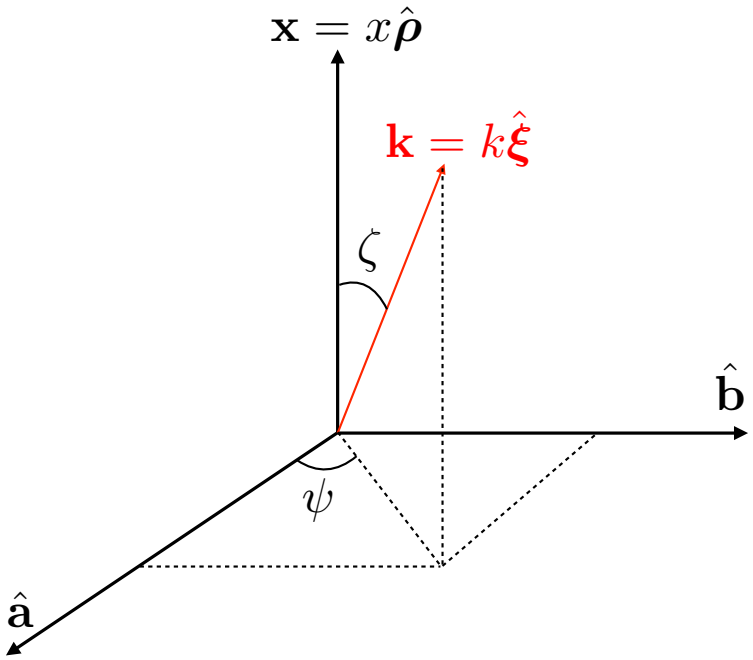

Figure 4.1: To illustrate the vectors and angles used to define $\mathbf{x}$ and $\mathbf{k}$.

At this point we recover the separation of variables in eqn.(4.9). Since $(kk) = k^2(\xi\xi)$ then the Fourier transform $\tilde{G}_{mp}(\mathbf{k})$ is given by:

$$\tilde{G}_{mp}(\mathbf{k}) = [(kk)^{-1}]_{mp} = \frac{1}{k^2}\left[(\xi\xi)^{-1}\right]_{mp},$$

where we recognise $1/k^2$ as being proportional to the Fourier transform of $1/x$ and the directional dependence of g_{mp} is contained in (the inverse transform of) $\left[(\xi\xi)^{-1}\right]_{mp}$. We note that since (kk) is symmetric, so is its inverse, and therefore $G_{mp}(\mathbf{x})$ is also symmetric, as required by the Maxwell reciprocity theorem. Since $\mathrm{d}^3k = k^2\sin\zeta\,\mathrm{d}k\,\mathrm{d}\zeta\,\mathrm{d}\psi$ and $\mathbf{k}\cdot\mathbf{x} = kx\cos\zeta$, eqn.(4.15) becomes:

$$G_{mp}(\mathbf{x}) = \frac{1}{(2\pi)^3}\int_0^{2\pi} d\psi \int_0^{\pi} d\zeta \sin\zeta \left[(\xi\xi)^{-1}\right]_{mp} \int_0^{\infty} dk \frac{1}{k^2} k^2 \cos(kx\cos\zeta).$$

The integration over k may be evaluated as follows:

$$\int_0^{\infty} dk \cos(kx\cos\zeta) = \frac{1}{2}\int_{-\infty}^{\infty} dk e^{ikx\cos\zeta} = \pi\delta(x\cos\zeta) = \frac{\pi}{x\sin\zeta}\delta(\zeta - \pi/2).$$

This simplifies the evaluation of $G_{mp}(\mathbf{x})$ considerably:

$$\begin{aligned} G_{mp}(\mathbf{x}) &= \frac{1}{(2\pi)^3}\int_0^{2\pi} d\psi \int_0^{\pi} d\zeta \cancel{\sin\zeta} \left[(\xi\xi)^{-1}\right]_{mp} \frac{\pi}{x\cancel{\sin\zeta}}\delta(\zeta - \pi/2) \\ &= \frac{1}{8\pi^2 x}\int_0^{2\pi} \left[(\xi\xi)^{-1}\right]_{mp} d\psi. \end{aligned} \tag{4.16}$$

The anticipated separation into radial $(1/x)$ and orientational dependencies is now explicit. The delta function $\delta(\zeta - \pi/2)$ requires that the integration with respect to ψ is around the unit circle perpendicular to the vector $\mathbf{x}$, with its centre at the origin. On this circle $\hat{\boldsymbol{\xi}} = \hat{\mathbf{a}}\cos\psi + \hat{\mathbf{b}}\sin\psi$. Thus, the orientational dependence of the Green's function resides in this line integral. In most cases of elastic anisotropy the line integral may be evaluated only numerically. But it is only one integral to be evaluated for each direction $\hat{\boldsymbol{\rho}}$, in contrast to the three integrals in the inverse Fourier transform of eqn.(4.15), and it is numerically stable. Finally, it is stressed that eqn.(4.16) is valid in *all* crystal symmetries. This remarkable result was first shown by J. L. Synge [9].

4.4 The elastic Green's function in an isotropic medium

In an isotropic medium the Green's function[10] can be determined directly by taking the inverse Fourier transform in eqn.(4.15).

Using eqn.(3.11) for the elastic constants in an isotropic elastic medium the matrix element $(kk)_{jm}$ is as follows:

$$(kk)_{jm} = \mu k^2 \delta_{jm} + (\lambda + \mu) k_j k_m \tag{4.17}$$

As we have seen in the previous section, the inverse of this matrix is the matrix of Fourier transforms $(kk)_{jm}\tilde{G}_{mp}(\mathbf{k}) = \delta_{jp}$. Rather than taking the brute force approach and evaluating the inverse of (kk) directly, we may multiply both sides of $(kk)_{jm}\tilde{G}_{mp}(\mathbf{k}) = \delta_{jp}$ by k_j and obtain an equation for $k_m\tilde{G}_{mp}(\mathbf{k})$:

[9] John Lighton Synge FRS (1897-1995). The derivation of eqn.(4.16) appears in his book *The hypercircle in mathematical physics* (1957) CUP: Cambridge, p.411-413.

[10] The solution in an isotropic medium for the displacement field of a point force was first derived by Lord Kelvin FRS in 1848, in a short paper entitled *Note on the integration of the equations of equilibrium of an elastic solid*, which can be found in Article 37 of Volume 1 of his *Mathematical and Physical Papers* p.97, available online at `https://archive.org/details/mathematicaland01kelvgoog`

$$k_m \tilde{G}_{mp}(\mathbf{k}) = \frac{k_p}{(\lambda+2\mu)k^2}$$

When this is substituted into $(\mu k^2 \delta_{jm} + (\lambda+\mu)k_j k_m)\tilde{G}_{mp}(\mathbf{k}) = \delta_{jp}$ we find:

$$\tilde{G}_{jp}(\mathbf{k}) = \frac{\delta_{jp}}{\mu k^2} - \frac{(\lambda+\mu)k_j k_p}{\mu(\lambda+2\mu)k^4} \tag{4.18}$$

It may be shown by contour integration that:

$$\begin{aligned} \int \frac{1}{k^2} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3 k &= \frac{2\pi^2}{x} \\ \int \frac{k_j k_p}{k^4} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3 k &= \pi^2 \left(\frac{\delta_{jp}}{x} - \frac{x_j x_p}{x^3} \right), \end{aligned}$$

where $x = |\mathbf{x}|$. Using these integrals to evaluate the inverse Fourier transform we obtain:

$$\begin{aligned} G_{jp}(\mathbf{x}) &= \frac{1}{8\pi\mu(\lambda+2\mu)x} \left((\lambda+3\mu)\delta_{jp} + (\lambda+\mu)\frac{x_j x_p}{x^2} \right) \\ &= \frac{1}{16\pi\mu(1-\nu)x} \left((3-4\nu)\,\delta_{jp} + \frac{x_j x_p}{x^2} \right) \end{aligned} \tag{4.19}$$

We shall use this result extensively.

Exercise 4.3 By fixing the value of x in eqn.(4.19) sketch the orientational dependencies of $G_{11}(\mathbf{x})$ and $G_{12}(\mathbf{x})$. ■

4.5 The multipole expansion

Consider a point defect in a crystal such as a foreign atom occupying a site that would normally be occupied by a host atom, i.e. a substitutional point defect. Let $\mathbf{f}^{(n)}$ be the excess force exerted on the n'th host atom when the site is occupied by the foreign atom as compared to when the site is occupied by a host atom. At equilibrium the net force on each atom is zero. But as we saw in section (2.4) the excess forces exerted by the defect on the host atoms in this equilibrium state are the source of the stress field it creates in the host. We call the excess force that the defect exerts on a host atom a 'defect force'. In this equilibrium state the defect may be viewed as a collection of defect forces that sum to zero because their sum is the negative of the net force on the defect atom, which is zero at equilibrium. The elastic displacement field generated by this collection of defect forces may be computed using the superposition principle and the elastic Green's function. This does involve approximations because the elastic Green's function and the superposition principle assume linear elasticity is valid. But beyond some distance from the defect the predicted displacement, stress and strain fields are expected to be accurate. Indeed, when we wish to calculate interaction energies between defects over distances much larger than the spatial extent of their defect forces, elasticity theory is very accurate. It provides also unrivalled physical insight into such interactions.

Let the foreign atom be located at $\mathbf{d}$. Let the position of the n'th neighbour relative to the foreign atom be $\mathbf{X}^{(n)}$, and let the defect force it experiences be $\mathbf{f}^{(n)}$. Therefore the displacement at $\mathbf{x}$ caused by the defect is:

$$u_i(\mathbf{x}) = \sum_n G_{ij}(\mathbf{x}-\mathbf{d}-\mathbf{X}^{(n)}) f_j^{(n)} \tag{4.20}$$

Within linear elasticity this is exact, but the approximations of linear elasticity are such that this expression becomes accurate only when $|\mathbf{x}-\mathbf{d}| \gg |\mathbf{X}^{(n)}|$. When this condition is satisfied we can expand the Green's function as a Taylor series:

$$G_{ij}(\mathbf{x}-\mathbf{d}-\mathbf{X}^{(n)}) = G_{ij}(\mathbf{x}-\mathbf{d}) - G_{ij,k}(\mathbf{x}-\mathbf{d})X_k^{(n)} + \frac{1}{2}G_{ij,kl}(\mathbf{x}-\mathbf{d})X_k^{(n)}X_l^{(n)} - \ldots$$

Inserting this expansion into eqn.(4.20) we obtain the following series:

$$\begin{aligned} u_i(\mathbf{x}) &= G_{ij}(\mathbf{x}-\mathbf{d})\sum_n f_j^{(n)} \\ &- G_{ij,k}(\mathbf{x}-\mathbf{d})\sum_n X_k^{(n)} f_j^{(n)} \\ &+ \frac{1}{2}G_{ij,kl}(\mathbf{x}-\mathbf{d})\sum_n X_k^{(n)}X_l^{(n)} f_j^{(n)} \\ &- \frac{1}{6}G_{ij,klm}(\mathbf{x}-\mathbf{d})\sum_n X_k^{(n)}X_l^{(n)}X_m^{(n)} f_j^{(n)} \ldots \end{aligned} \tag{4.21}$$

This equation is called the multipole expansion of the displacement field of a point defect. At equilibrium the first term on the right hand side of eqn.(4.21) is zero because the defect forces sum to zero. The next term involves the first moment of the defect forces, which is called the elastic dipole tensor: $\rho_{kj} = \sum_n X_k^{(n)} f_j^{(n)}$. The next term involves the second moment of the defect forcesr, $q_{klj} = \sum_n X_k^{(n)} X_l^{(n)} f_j^{(n)}$ and is called the elastic quadrupole tensor. The next term involves the third moment of the defect forces $o_{klmj} = \sum_n X_k^{(n)} X_l^{(n)} X_m^{(n)} f_j^{(n)}$, and is called the elastic octopole tensor, and so on.

Exercise 4.4 Equilibrium requires not only that the net force on the point defect is zero but also that the net torque exerted on the defect atom is zero. Show that this condition is satisfied provided the elastic dipole tensor is symmetric: $\rho_{ij} = \rho_{ji}$. ∎

The multipole expansion reveals how the elastic displacement field of a point defect decays with distance x. The dipole tensor gives rise to a displacement field that decays as $1/x^2$, the quadrupole as $1/x^3$, the octopole as $1/x^4$ and so on. The displacement fields from higher oder poles become increasingly significant as the defect is approached. The orientational dependence of each of these contributions to the displacement field is contained in the derivatives of the Green's functions.

The multipole expansion reflects the symmetry of the atomic environment surrounding the point defect. This is very significant for those point defects that have particular symmetries, such as crowdions which have a distinct axial symmetry.

Finally, we note that eqn.(4.21) is an exemplar of 'multi-scale modelling'. It takes information from the atomic scale, namely the defect forces, and applies the theory of elasticity to determine the elastic field of the point defect at long range. It is a bridge between the atomic and continuum length

scales, and perhaps this is why it was described by Leibfried and Breuer as 'without exaggeration, the most important new concept needed in defect physics'[11]. Kröner[12] was the first to introduce a systematic description of point defects in terms of force multipoles[13].

4.6 Relation between the elastic and crystal lattice Green's functions

Consider a crystal containing N lattice sites, with one atom at each lattice site. In harmonic lattice theory the potential energy of the distorted crystal is expanded to second order in the displacements of atoms from their perfect crystal positions. Using a slightly different notation from eqn.(3.28) the potential energy is as follows:

$$E = -\sum_n f_i(\mathbf{X}^{(n)})u_i(\mathbf{X}^{(n)}) + \frac{1}{2}\sum_n\sum_p S_{ij}(\mathbf{X}^{(n)} - \mathbf{X}^{(p)})u_i(\mathbf{X}^{(n)})u_j(\mathbf{X}^{(p)}). \tag{4.22}$$

We have replaced $u_i^{(n)}$ and $S_{ij}^{(np)}$ in eqn.(3.28) with $u_i(\mathbf{X}^{(n)})$ and $S_{ij}(\mathbf{X}^{(n)} - \mathbf{X}^{(p)})$ respectively. The force $f_i(\mathbf{X}^{(n)})$ is not zero this time because now there is a crystal defect that displaces the atom from its perfect crystal position at $\mathbf{X}^{(n)}$. It is equivalent to the body forces we have discussed in elasticity. This is different from eqn.(3.28), where the forces were all set to zero, because the perfect crystal configuration was being considered with no defects present.

By minimising the energy in eqn.(4.22) with respect to the displacements we obtain the following equation:

$$f_m(\mathbf{X}^{(n)}) = \sum_p S_{mj}(\mathbf{X}^{(n)} - \mathbf{X}^{(p)})u_j(\mathbf{X}^{(p)}). \tag{4.23}$$

We want the inverse of this relationship, that is we want an expression for the displacements in terms of the forces:

$$u_l(\mathbf{X}^{(n)}) = \sum_p G_{lh}(\mathbf{X}^{(n)} - \mathbf{X}^{(p)})f_h(\mathbf{X}^{(p)}) \tag{4.24}$$

This equation is equivalent in the discrete lattice to eqn.(4.6) in the continuum, and it defines the crystal lattice Green's function. In this section we investigate the relationship between this crystal lattice Green's function and the elastic Green's function. To invert eqn.(4.23) we use discrete Fourier transforms defined by:

$$\tilde{W}(\mathbf{k}) = \sum_n W(\mathbf{X}^{(n)})e^{i\mathbf{k}\cdot\mathbf{X}^{(n)}} \tag{4.25}$$

$$W(\mathbf{X}^{(p)}) = \frac{1}{N}\sum_{\mathbf{k}} \tilde{W}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{X}^{(p)}}. \tag{4.26}$$

Born von Karman periodic boundary conditions are applied to the crystal faces, and there are N wave vectors $\mathbf{k}$ in the Brillouin zone. Taking the discrete Fourier transform of eqn.(4.23) we obtain:

$$\tilde{f}_m(\mathbf{k}) = \tilde{S}_{mj}(\mathbf{k})\tilde{u}_j(\mathbf{k}), \tag{4.27}$$

[11] G Leibfried and N. Breuer, *Point defect in Metals I*, Springer-Verlag: Berlin, p.146 (1978)

[12] Ekkehart Kröner (1919-2000)

[13] E. Kröner *Kontinuumstheorie der Versetzungen und Eigenspannungen*, Springer-Verlag: Berlin (1958)

where $\tilde{S}_{mj}(\mathbf{k})$ is a 3×3 matrix for each wave vector $\mathbf{k}$ in the Brillouin zone. Inverting this equation we obtain:

$$\tilde{u}_l(\mathbf{k}) = \left[\tilde{S}^{-1}(\mathbf{k})\right]_{lh}\tilde{f}_h(\mathbf{k}). \tag{4.28}$$

Taking the discrete inverse Fourier transform we find:

$$\begin{aligned} u_l(\mathbf{X}^{(n)}) &= \frac{1}{N}\sum_{\mathbf{k}}\left[\tilde{S}^{-1}(\mathbf{k})\right]_{lh}\tilde{f}_h(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{X}^{(n)}} \\ &= \frac{1}{N}\sum_{\mathbf{k}}\left[\tilde{S}^{-1}(\mathbf{k})\right]_{lh}\left(\sum_p f_h(\mathbf{X}^{(p)})e^{i\mathbf{k}\cdot\mathbf{X}^{(p)}}\right)e^{-i\mathbf{k}\cdot\mathbf{X}^{(n)}} \\ &= \sum_p\left(\frac{1}{N}\sum_{\mathbf{k}}\left[\tilde{S}^{-1}(\mathbf{k})\right]_{lh}e^{-i\mathbf{k}\cdot(\mathbf{X}^{(n)}-\mathbf{X}^{(p)})}\right)f_h(\mathbf{X}^{(p)}) \end{aligned}$$

Comparing this with eqn.(4.24) we obtain the desired expression for the crystal lattice Green's function:

$$G_{lh}(\mathbf{X}^{(n)}-\mathbf{X}^{(p)}) = \frac{1}{N}\sum_{\mathbf{k}}\left[\tilde{S}^{-1}(\mathbf{k})\right]_{lh}e^{-i\mathbf{k}\cdot(\mathbf{X}^{(n)}-\mathbf{X}^{(p)})}. \tag{4.29}$$

To aid comparison we quote here the elastic Green's function from eqn.(4.15):

$$G_{mp}(\mathbf{x}) = \frac{1}{(2\pi)^3}\int\left[(kk)^{-1}\right]_{mp}e^{-i\mathbf{k}\cdot\mathbf{x}}\,\mathrm{d}^3k$$

Since $S_{mj}(\mathbf{X}^{(n)}) = S_{mj}(-\mathbf{X}^{(n)})$, and $\sum_n S_{mj}(\mathbf{X}^{(n)}) = 0$, we may write[14]:

$$\begin{aligned} \tilde{S}_{mj}(\mathbf{k}) &= \sum_n S_{mj}(\mathbf{X}^{(n)})e^{i\mathbf{k}\cdot\mathbf{X}^{(n)}} \\ &= \frac{1}{2}\sum_n S_{mj}(\mathbf{X}^{(n)})\left(e^{i\mathbf{k}\cdot\mathbf{X}^{(n)}}+e^{-i\mathbf{k}\cdot\mathbf{X}^{(n)}}-2\right) \\ &= \frac{1}{2}\sum_n S_{mj}(\mathbf{X}^{(n)})\left(2\cos\left(\mathbf{k}\cdot\mathbf{X}^{(n)}\right)-2\right) \\ &= -2\sum_n S_{mj}(\mathbf{X}^{(n)})\sin^2\left(\frac{\mathbf{k}\cdot\mathbf{X}^{(n)}}{2}\right) \end{aligned}$$

In the limit of long wavelengths the magnitude of the wave vector $\mathbf{k}$ becomes very small. In that limit we may write:

$$\begin{aligned} \tilde{S}_{mj}(\mathbf{k}) &\to -\frac{1}{2}\sum_n S_{mj}(\mathbf{X}^{(n)})(\mathbf{k}\cdot\mathbf{X}^{(n)})^2 \\ &= \left[-\frac{1}{2}\sum_n S_{mj}(\mathbf{X}^{(n)})X_h^{(n)}X_l^{(n)}\right]k_hk_l. \end{aligned}$$

[14] see *Solid state physics* by N W Ashcroft and N D Mermin (1976), p437-440

Comparing with the expression for the elastic constant tensor c_{ikjl} in eqn.(3.31) we recognise the term in square brackets as being Ωc_{mhjl}, and therefore in the limit of long wavelengths $\tilde{S}_{mj}(\mathbf{k}) \to \Omega(kk)_{mj}$.

Each $\mathbf{k}$-point in the Brillouin zone is associated with a volume in $\mathbf{k}$-space of $(2\pi)^3/(N\Omega)$. Replacing the sum over $\mathbf{k}$-points in eqn.(4.29) with a continuous integral over all $\mathbf{k}$-space we find the crystal lattice Green's function, in the limit of long wavelengths, becomes:

$$G_{mp}(\mathbf{X}^{(n)}) \to \frac{1}{N\Omega}\frac{N\Omega}{(2\pi)^3}\int \mathrm{d}^3k \left[(kk)^{-1}\right]_{mp} e^{-i\mathbf{k}\cdot\mathbf{X}^{(n)}} = \frac{1}{(2\pi)^3}\int \mathrm{d}^3k \left[(kk)^{-1}\right]_{mp} e^{-i\mathbf{k}\cdot\mathbf{X}^{(n)}}, \quad (4.30)$$

which is identical to the elastic Green's function. We conclude that the elastic and crystal lattice Green's functions are equivalent only in the limit of long wavelengths compared to the distance from the force creating the displacement, so that $\mathbf{k}\cdot\mathbf{x} \ll 1$. At smaller wavelengths the lattice Green's function may be expected to deviate significantly from the elastic Green's function. The implication is that when we are studying the elastic displacement fields of defects with the elastic Green's function the fields nearer to the defect are less accurate than those further away. At larger distances from the defect the smaller wavelength contributions to the crystal lattice Green's function tend to cancel out, leaving only the longer wavelength components.

4.7 The equation of motion and elastic waves

We shall use Hamilton's principle of classical mechanics[15] to derive the equation of motion of the continuum. Hamilton's principle states that the following integral is stationary with respect to variations δu_i of the displacement field which vanish at times $t = t_1$ and $t = t_2$ and on the surface of the volume V:

$$\delta \int_{t_1}^{t_2} \mathrm{d}t \int_V \mathrm{d}V \mathscr{L}(u_i, \dot{u}_i, u_{i,j}) = 0. \quad (4.31)$$

$\mathscr{L}$ is the Lagrangian density, which is the difference between the kinetic energy and the potential energy densities:

$$\mathscr{L} = \frac{1}{2}\rho\dot{u}_i^2 - \left(-f_i u_i + \frac{1}{2}c_{ijkl}u_{i,j}u_{k,l}\right).$$

In this expression ρ is the mass density, $\dot{u}_i$ is the velocity of the medium at $\mathbf{x}$, and we have included a contribution from body forces f_i in the potential energy density. Substituting this Lagrangian density into eqn.(4.31) and performing the variation we obtain:

$$\begin{aligned}
\delta \int_{t_1}^{t_2} \mathrm{d}t \int_V \mathrm{d}V \mathscr{L}(u_i, \dot{u}_i, u_{i,j}) &= \int_{t_1}^{t_2} \mathrm{d}t \int_V \mathrm{d}V\ \rho\dot{u}_i\delta\dot{u}_i + f_i\delta u_i - c_{ijkl}u_{i,j}\delta u_{k,l} \\
&= \int_V \mathrm{d}V [\rho\dot{u}_i\delta u_i]_{t=t_1}^{t_2} - \int_{t_1}^{t_2}\mathrm{d}t\int_V \mathrm{d}V\rho\ddot{u}_i\delta u_i - f_i\delta u_i + \left(c_{ijkl}u_{i,j}\delta u_k\right)_{,l} - c_{ijkl}u_{i,jl}\delta u_k \\
&= -\int_{t_1}^{t_2}\int_S c_{ijkl}u_{i,j}\delta u_k n_l \mathrm{d}S - \int_{t_1}^{t_2}\mathrm{d}t\int_V \mathrm{d}V\left(\rho\ddot{u}_i - f_i - \sigma_{ij,j}\right)\delta u_i
\end{aligned} \quad (4.32)$$

[15] for example, see H. Goldstein *Classical mechanics*, Addison-Wesley: Reading Mass. (1980)

We have used $\delta u_i = 0$ at $t = t_1$ and $t = t_2$, and on the surface S of the body at all times. We have also used the divergence theorem to convert a volume integral into a surface integral. In order for the variation to be zero the integrand must be zero:

$$\rho \ddot{u}_i = f_i + \sigma_{ij,j}, \tag{4.33}$$

which is the equation of motion of the continuum.

4.7.1 Elastic waves

In the absence of forces in the equation of motion, eqn.(4.33), we try a wave solution of the form $u_i(\mathbf{x},t) = A_i(\mathbf{k},\omega)e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$, which leads to the equation:

$$\left(\rho\omega^2\delta_{ij} - (kk)_{ij}\right)A_j(\mathbf{k},\omega) = 0. \tag{4.34}$$

This is a set of three equations in the wave amplitudes $A_i(\mathbf{k},\omega)$, and the condition for non-trivial solutions is that the following 3×3 determinant is zero:

$$\begin{vmatrix} (kk)_{11}-\rho\omega^2 & (kk)_{12} & (kk)_{13} \\ (kk)_{12} & (kk)_{22}-\rho\omega^2 & (kk)_{23} \\ (kk)_{13} & (kk)_{23} & (kk)_{33}-\rho\omega^2 \end{vmatrix} = 0. \tag{4.35}$$

In general this provides a set of three solutions for $\omega^2 = \omega^2(\mathbf{k})$, which are known as the three branches of the dispersion relations. By writing $(kk) = k^2(\xi\xi)$ and by making ω/k the quantity to be determined the determinant can be rewritten as follows:

$$\begin{vmatrix} (\xi\xi)_{11}-\rho\omega^2/k^2 & (\xi\xi)_{12} & (\xi\xi)_{13} \\ (\xi\xi)_{12} & (\xi\xi)_{22}-\rho\omega^2/k^2 & (\xi\xi)_{23} \\ (\xi\xi)_{13} & (\xi\xi)_{23} & (\xi\xi)_{33}-\rho\omega^2/k^2 \end{vmatrix} = 0. \tag{4.36}$$

This makes it clear that ω is a linear function of k and that ω varies in general with the direction of $\mathbf{k}$. Thus, in general, the group velocity of the wave, $\mathbf{v}_g = \nabla_{\mathbf{k}}\omega(\mathbf{k})$, depends on the direction of the wave but not on its frequency. In particular, we note that in general the wave does not travel in the direction of its wave vector because in general $\mathbf{v}_g$ is not parallel to $\mathbf{k}$. Since the $(\xi\xi)$ matrix is symmetric its eigenvalues are always real and its eigenvectors are always perpendicular to each other. The eigenvectors are the amplitudes $\mathbf{A}(\mathbf{k},\omega)$ in eqn.(4.34) and their directions relative to the wave vector $\mathbf{k}$ determine whether the waves are longitudinal or transverse or a mixture of the two.

In the isotropic elastic approximation (kk) is given by eqn.(4.17). One solution of the dispersion equations, eqn.(4.35), is $c_l^2 = \omega^2/k^2 = (\lambda+2\mu)/\rho$, and is independent of the direction of $\mathbf{k}$, as expected in an isotropic medium. When this solution is substituted back into eqn.(4.34) it is found the wave amplitude is parallel to the wave vector and it is called the longitudinal wave or 'P-wave'. This wave produces alternating compression and dilation of the medium along the direction of propagation of the wave. The other two solutions are degenerate with $c_t^2 = \omega^2/k^2 = \mu/\rho$, and they are also independent of the direction of the wave vector. In these cases the wave amplitudes are perpendicular to each other and to the wave vector, and they are called transverse waves, or 'S-waves'. These waves produce shears of the medium and are not associated with local volume

changes. For all three waves the group velocity is always parallel to the wave vector, and there is always one purely longitudinal wave and two purely transverse waves for all wave vectors. This combination of features of the propagation of elastic waves in isotropic materials is unique, and may be found in anisotropic materials only when the wave vector coincides with a direction of high rotational symmetry.

4.8 The elastodynamic Green's function

Having analysed the properties of elastic waves we are in a position to tackle the time-dependent Green's function of elastodynamics. The time-dependent generalisation of eqn.(4.8) for the elastostatic Green's function is to consider a point force that is applied as an infinitely abrupt pulse at $t = 0$ that generates a displacement field that propagates away. In an isotropic medium we can expect a spherical longitudinal wave to travel outwards from the point pulse followed by two degenerate spherical shear waves. Thus in the equation of motion, eqn.(4.33), we set $f_i = \delta_{im}\delta(\mathbf{x})\delta(t)$ to describe a pulse of force of unit magnitude along the x_m axis at the origin at time $t = 0$. The elastodynamic Green's function in an infinite, homogeneous elastic medium is then defined by the following partial differential equation:

$$c_{ijkl}G_{km,lj}(\mathbf{x},t) + \delta_{im}\delta(\mathbf{x})\delta(t) = \rho\ddot{G}_{im}(\mathbf{x},t) \tag{4.37}$$

To solve this equation we exploit the translational symmetry of the medium in space and time through four-dimensional Fourier transforms:

$$\tilde{f}(\mathbf{k},\omega) = \int\int f(\mathbf{x},t)\, e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}\, \mathrm{d}^3x\,\mathrm{d}t \tag{4.38}$$

$$f(\mathbf{x},t) = \frac{1}{(2\pi)^4}\int\int \tilde{f}(\mathbf{k},\omega)\, e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega t)}\, \mathrm{d}^3k\,\mathrm{d}\omega \tag{4.39}$$

Applying the four-dimensional Fourier transform to eqn.(4.37) we obtain:

$$\left((kk)_{ik} - \rho\omega^2\delta_{ik}\right)\tilde{G}_{km}(\mathbf{k},\omega) = \delta_{im}, \tag{4.40}$$

from which it follows that

$$G_{km}(\mathbf{x},t) = \int\int \left[\left((kk) - \rho\omega^2 I\right)^{-1}\right]_{km} e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega t)}\, \mathrm{d}^3k\,\mathrm{d}\omega$$

where I is the 3×3 identity matrix.

As with the elastostatic Green's function we resort to the isotropic elastic approximation to make further progress[16] whereupon we have:

$$\left((kk) - \rho\omega^2 I\right)_{ik} = (\mu k^2 - \rho\omega^2)\delta_{ik} + (\lambda+\mu)k_i k_k$$

[16]This was first done by Sir George G. Stokes PRS (1819-1903) in his paper *On the dynamical theory of diffraction*, Trans. Camb. Phil. Soc. **9** (1849), 1-62, available online at `https://archive.org/stream/transactionsofca09camb`

Exercise 4.5 Using the same procedure to invert (kk) following eqn.(4.17) show that

$$\tilde{G}_{im}(\mathbf{k},\omega) = \left[((kk)-\rho\omega^2 I)^{-1}\right]_{im} = \frac{1}{\rho}\left[\frac{\delta_{im}-k_ik_m/k^2}{c_t^2k^2-\omega^2}+\frac{k_ik_m/k^2}{c_l^2k^2-\omega^2}\right]$$

■

Taking the inverse Fourier transform we obtain the following Green's function for $t>0$ for the point force pulse at the origin:

$$\begin{aligned} 4\pi\rho x G_{ij}(\mathbf{x},t) &= \frac{\delta(x-c_lt)}{c_l}\frac{x_ix_j}{x^2}+\frac{\delta(x-c_tt)}{c_t}\left(\delta_{ij}-\frac{x_ix_j}{x^2}\right) \\ &+ [H(x-c_lt)-H(x-c_tt)]\frac{t}{x^2}\left(\delta_{ij}-\frac{3x_ix_j}{x^2}\right), \end{aligned} \tag{4.41}$$

where $H(x)$ is the Heaviside step function: $H(x)=1$ if $x>0$, $H(x)=0$ if $x<0$. We see in this solution two spherical waves emanating from the point force pulse at the origin, with the longitudinal wave expanding faster than the shear wave. The material beyond the longitudinal wave front is undeformed.

4.9 Problem Set 4

1. Derive the isotropic elastic Green's function using the line integral in eqn.(4.16).

2. A *dumb-bell* interstitial defect[17] has axial symmetry and is located at the origin of a Cartesian coordinate system in an elastically isotropic medium. With its axis along the unit vector $\hat{\mathbf{e}}$ it exerts a defect force $f\hat{\mathbf{e}}$ at $h\hat{\mathbf{e}}$ and another defect force $-f\hat{\mathbf{e}}$ at $-h\hat{\mathbf{e}}$.

   Write down the dipole tensor for the defect.

   Show that in an isotropic medium

   $$G_{ij,k}(\mathbf{x}) = \frac{-1}{16\pi\mu(1-\nu)x^2}\left((3-4\nu)\rho_k\delta_{ij}-(\rho_j\delta_{ik}+\rho_i\delta_{jk})+3\rho_i\rho_j\rho_k\right), \tag{4.42}$$

   where $\rho_i = x_i/x$.

   Hence show that for $x \gg h$ the displacement field at $\mathbf{x}$ of the dumb-bell defect is given by

   $$u_i(\mathbf{x}) = \frac{2fh}{16\pi\mu(1-\nu)x^2}\left[(3\cos^2\alpha-1)\rho_i+2(1-2\nu)(\cos\alpha)e_i\right]$$

   where $\cos\alpha = e_j\rho_j$.

   Hence show that at a given distance x from the point defect the elastic displacement along the axis of the defect is $4(1-\nu)$ larger than the displacement along any direction perpendicular to the defect axis, and of opposite sign.

[17] An interstitial defect occupies a site between those of the host crystal. The defect force for an interstitial defect is therefore the entire force it exerts on a neighbour in the relaxed configuration.

3. Consider a cubic crystal where the elastic anisotropy ratio is close to 1. Then $D = c_{11} - c_{12} - 2c_{44}$ is small compared to c_{12} and c_{44}. Eqn.(3.22) for the elastic constant tensor in a cubic crystal may always be expressed as

$$c_{ijkl} = c^0_{ijkl} + \delta_{ijkl} D,$$

where c^0_{ijkl} is the elastic constant tensor for an isotropic crystal where we choose $c^0_{12} = c_{12} = \lambda$, $c^0_{44} = c_{44} = \mu$, and as before $\delta_{ijkl} = 1$ if $i = j = k = l$, zero otherwise. Let $(KK)_{jm} = c_{jlms} k_l k_s$ and $(kk)_{jm} = c^0_{jlms} k_l k_s$. Show that:

$$(KK)^{-1} = (kk)^{-1} - (kk)^{-1} V (KK)^{-1},$$

where $V_{jm} = D(k_1^2 \delta_{j1}\delta_{m1} + k_2^2 \delta_{j2}\delta_{m2} + k_3^2 \delta_{j3}\delta_{m3})$. This equation[18] is exact whatever the magnitude of D. Although it can be solved for $(KK)^{-1}$ the inverse Fourier transform requires the solution of a sextic equation to locate the poles, which can be done only numerically. However, since D/μ is small it suggests a perturbation expansion:

$$(KK)^{-1} = (kk)^{-1} - (kk)^{-1} V (kk)^{-1} + (kk)^{-1} V (kk)^{-1} V (kk)^{-1} - \ldots$$

Using eqn.(4.18) for $\left[(kk)^{-1}\right]_{jp}$ show that to first order in D/c_{44} the Green's function tensor in the cubic crystal in k-space becomes:

$$\begin{aligned}
&\tilde{G}_{ij}(\mathbf{k}) = \left[(KK)^{-1}\right]_{ij} = \\
&\frac{1}{\mu}\frac{\delta_{ij}}{k^2} - \frac{1}{\mu}\left(\frac{\lambda+\mu}{\lambda+2\mu}\right)\frac{k_i k_j}{k^4} \\
&+\frac{D}{\mu}\frac{1}{\mu}\frac{\left(\delta_{i1}k_1^2\delta_{j1} + \delta_{i2}k_2^2\delta_{j2} + \delta_{i3}k_3^2\delta_{j3}\right)}{k^4} \\
&-\frac{D}{\mu}\frac{1}{\mu}\left(\frac{\lambda+\mu}{\lambda+2\mu}\right)\frac{\left(k_1^3(\delta_{i1}k_j + k_i\delta_{j1}) + k_2^3(\delta_{i2}k_j + k_i\delta_{j2}) + k_3^3(\delta_{i3}k_j + k_i\delta_{j3})\right)}{k^6} \\
&+\frac{D}{\mu}\frac{1}{\mu}\left(\frac{\lambda+\mu}{\lambda+2\mu}\right)^2 k_i k_j \frac{(k_1^4 + k_2^4 + k_3^4)}{k^8}
\end{aligned} \tag{4.43}$$

Hence show that the first order corrections to the isotropic elastic Green's functions are:

$$\begin{aligned}
\Delta\tilde{G}_{11}(\mathbf{k}) &= \frac{D}{\mu}\frac{1}{\mu}\left(\frac{k_1^2}{k^4} - \chi\frac{2k_1^4}{k^6} + \chi^2\frac{k_1^2(k_1^4 + k_2^4 + k_3^4)}{k^8}\right) \\
\Delta\tilde{G}_{12}(\mathbf{k}) &= \frac{D}{\mu}\frac{1}{\mu}\left(-\chi\frac{k_1^3 k_2 + k_1 k_2^3}{k^6} + \chi^2\frac{k_1 k_2(k_1^4 + k_2^4 + k_3^4)}{k^8}\right)
\end{aligned}$$

where $\chi = (\lambda+\mu)/(\lambda+2\mu)$.

To invert these Fourier transforms the following integral, which may be obtained by contour integration, is useful:

[18] This is a Dyson equation - see E. N. Economou *Green's functions in quantum physics*, Springer-Verlag: Berlin (1983).

$$\frac{1}{(2\pi)^3}\int \frac{1}{k^{2n}} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3k = -\frac{1}{4\pi}\frac{i^{2n}x^{2n-3}}{(2n-2)!}\,,$$

where $n = 1,2,3,\ldots$. Other integrals needed to evaluate the inverse transforms may by obtained by differentiating this one with respect to components of $\mathbf{x}$. In this way we may obtain the following inverse transforms:

$$\begin{aligned}
\frac{1}{(2\pi)^3}\int \frac{k_1^2}{k^4} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3k &= -\frac{1}{8\pi x}\left(1-\frac{x_1^2}{x^2}\right)\\
\frac{1}{(2\pi)^3}\int \frac{k_1^3k_j}{k^6} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3k &= \frac{3}{32\pi x}\left(\delta_{1j}-\frac{x_1x_j}{x^2}\right)\left(1-\frac{x_1^2}{x^2}\right)\\
\frac{1}{(2\pi)^3}\int \frac{k_1^5k_j}{k^8} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3k &= \frac{5}{64\pi x}\left(\delta_{1j}-\frac{x_1x_j}{x^2}\right)\left(1-\frac{x_1^2}{x^2}\right)^2\\
\frac{1}{(2\pi)^3}\int \frac{k_1^2k_2^4}{k^8} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3k &= \frac{1}{64\pi x}\left(1-\frac{x_2^2}{x^2}\right)\left(\frac{x_3^2}{x^2}+5\frac{x_1^2x_2^2}{x^4}\right)\\
\frac{1}{(2\pi)^3}\int \frac{k_1k_2k_3^4}{k^8} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}^3k &= -\frac{1}{64\pi x}\frac{x_1x_2}{x^2}\left(1-\frac{x_3^2}{x^2}\right)\left(1-5\frac{x_3^2}{x^2}\right)
\end{aligned}$$

Hence show that:

$$\begin{aligned}
\Delta G_{11}(\mathbf{x}) = \frac{1}{\mu}\frac{D}{\mu}\frac{1}{8\pi x}\Bigg[&-\left(1-\frac{x_1^2}{x^2}\right)-\frac{3\chi}{2}\left(1-\frac{x_1^2}{x^2}\right)^2\\
&+\frac{\chi^2}{8}\left(5\left(1-\frac{x_1^2}{x^2}\right)^3+\left(1-\frac{x_2^2}{x^2}\right)\left(\frac{x_3^2}{x^2}+5\frac{x_1^2x_2^2}{x^4}\right)+\left(1-\frac{x_3^2}{x^2}\right)\left(\frac{x_2^2}{x^2}+5\frac{x_1^2x_3^2}{x^4}\right)\right)\Bigg]
\end{aligned}$$

$$\begin{aligned}
\Delta G_{12}(\mathbf{x}) = \frac{1}{\mu}\frac{D}{\mu}\frac{1}{8\pi x}\frac{x_1x_2}{x^2}\Bigg[&\frac{3\chi}{4}\left(1+\frac{x_3^2}{x^2}\right)\\
&-\frac{\chi^2}{8}\left(5\left(\left(1-\frac{x_1^2}{x^2}\right)^2+\left(1-\frac{x_2^2}{x^2}\right)\right)+\left(1-\frac{x_3^2}{x^2}\right)\left(1-5\frac{x_3^2}{x^2}\right)\right)\Bigg]
\end{aligned}$$

The other elements of the Green's function are found by permuting the subscripts.

4. In a hexagonal crystal show that the (kk) matrix is as follows:

$$(kk) = \begin{bmatrix} c_{11}k_1^2+c_{66}k_2^2+c_{44}k_3^2 & \frac{1}{2}(c_{11}+c_{12})k_1k_2 & (c_{44}+c_{13})k_1k_3\\ \frac{1}{2}(c_{11}+c_{12})k_1k_2 & c_{66}k_1^2+c_{11}k_2^2+c_{44}k_3^2 & (c_{44}+c_{13})k_2k_3\\ (c_{44}+c_{13})k_1k_3 & (c_{44}+c_{13})k_2k_3 & c_{44}(k_1^2+k_2^2)+c_{33}k_3^2 \end{bmatrix}$$

where $c_{66} = \frac{1}{2}(c_{11}-c_{12})$.

Since the elastic constant tensor is invariant with respect to rotations about the hexagonal axis (which is the x_3-axis), we may choose $\mathbf{k} = (0,k_2,k_3)$. With this simplification the determinant

in eqn.(4.35) can be factorised. Determine the three solutions for $\omega^2 = \omega^2(0,k_2,k_3)$.

Determine the frequencies and polarisations of the three waves with $\mathbf{k}$ in the basal plane and normal to the basal plane.

5. Consider the Green's function, $\gamma_{km}(\mathbf{x},t)$, for an oscillatory unit body force located at the origin described by $f_i(t) = \delta_{im}\delta(\mathbf{x})\cos(\omega t)$. The equation of motion for $\gamma_{km}(\mathbf{x},t)$ is as follows:

$$c_{ijkl}\gamma_{km,lj}(\mathbf{x},t) + \delta_{im}\delta(\mathbf{x})\cos(\omega t) = \rho\,\ddot{\gamma}_{im}(\mathbf{x},t).$$

To satisfy the time dependence in this equation we must have[19] $\gamma_{im}(\mathbf{x},t) = \chi_{im}(\mathbf{x})\cos\omega t$, where $\chi(\mathbf{x})$ satisfies following equation:

$$c_{ijkl}\chi_{km,lj}(\mathbf{x}) + \delta_{im}\delta(\mathbf{x}) = -\rho\,\omega^2\chi_{im}(\mathbf{x})$$

Show that the Fourier transform $\tilde{\chi}(\mathbf{k})$satisfies:

$$\left[(kk)_{ik} - \rho\,\omega^2\delta_{ik}\right]\tilde{\chi}_{km} = \delta_{im}$$

and therefore

$$\tilde{\chi}_{im} = \frac{1}{\rho}\left[\frac{\delta_{im} - k_i k_m/k^2}{c_t^2 k^2 - \omega^2} + \frac{k_i k_m/k^2}{c_l^2 k^2 - \omega^2}\right].$$

Hence show that

$$\chi_{im}(\mathbf{x}) = \frac{\delta_{im}}{\rho c_t^2}\frac{\cos(\omega x/c_t)}{2\pi x} + \frac{1}{\rho\,\omega^2}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_m}\left(\frac{\cos(\omega x/c_t) - \cos(\omega x/c_l)}{2\pi x}\right).$$

[19] if damping were included in the equation of motion there would be a phase difference between the vibrations of the medium and those of the oscillator.

5. Point defects

The theory perhaps suffers from the disadvantage that its limitations are more immediately obvious than are those of other approximate methods which have to be used in dealing with the solid state. ... A simple treatment at cottage-industry level may sometimes provide a certain degree of insight into some phenomenon or other when an exact calculation, based on a theoretical model which apes reality precisely, will give accurate answers but may be too unsurveyable, or too numerical, to give much insight.

J. D Eshelby[1] (1977). In *Point defect behaviour and diffusional processes*, eds. R. E. Smallman and E. Harris, pp.3-10, The Metals Society, London.

5.1 Introduction

Point defects are ubiquitous in crystalline materials. They are classified as either intrinsic or extrinsic. Intrinsic point defects are vacancies and self-interstitials. A vacancy is a vacant atomic site that would normally be occupied by a host atom. A self-interstitial is created when one of the atoms of the crystal is occupying a site in the space, called the the 'interstice', between usual crystal sites. Extrinsic point defects are foreign atoms that have been incorporated into the crystal structure either on substitutional or interstitial sites.

Unlike linear and planar defects there may be populations of point defects in thermodynamic equilibrium in a crystal. For example the equilibrium concentration of vacancies in a crystal at a given temperature and pressure is $\exp(-G^f/k_BT)$ where G^f is the Gibbs free energy of formation of the point defect, k_B is the Boltzmann constant and T is temperature. The thermodynamic equilibrium concentration of foreign atoms in a crystal depends on their chemical potentials, which in turn depend on the partial pressures of these impurities in the vapour phase in equilibrium with the crystal.

Thermodynamic equilibrium is seldom achieved in crystals, but its existence is important because it indicates the state of the system towards which it will naturally evolve under prescribed

[1] John D. Eshelby, FRS (1916-1981)

environmental conditions provided it is not being driven away from thermodynamic equilibrium by external influences such as mechanical deformation or irradiation. The diffusion of point defects leads to mass transport and possibly changes of phase in the solid state. For example diffusion in pure crystals usually occurs through the migration of vacancies, as they are the only sites in the crystal that can undergo a change of occupation through a host atom jumping into it. This is analogous to electronic conduction in a p-type semiconductor which occurs through the movement of electronic holes at the top of the valence band.

Point defects may be created in concentrations far in excess of those prescribed by thermodynamic equilibrium through processes such as plastic deformation and irradiation by high energy particles. When this happens the point defects may aggregate and form small interstitial and vacancy clusters that can be very mobile, especially when they are small. Intrinsic point defects such as vacancies may be attracted to foreign atoms and form new combined defects called complexes. The variety of point defects can be huge.

In this chapter we will focus on how point defects interact with each other through their elastic fields. We begin with the model of a point defect as a misfitting sphere. We will go on to consider models of point defects that capture the symmetry of the atomic environment of the point defect.

5.2 The misfitting sphere model of a point defect

The simplest model of a point defect is a misfitting sphere[2] due to Bilby[3]. Cut out a spherical hole of radius r_h in an elastic continuum. Insert into the hole a sphere of radius $r_s \neq r_h$ and weld the interface. The sphere may be larger or smaller than the hole. We consider first the case where the inserted sphere is rigid and the continuum is infinite in extent. All the deformation occurs in the continuum surrounding the sphere.

Let $\mathbf{u}^\infty(\mathbf{r})$ be the displacement field in the continuum surrounding the sphere at radius r. The superscipt 'infinity' is to remind us that the continuum is infinite in extent. The displacement field will be purely radial so that $\mathbf{u}^\infty(\mathbf{r}) = \mathbf{u}^\infty(|\mathbf{r}|) = \mathbf{u}^\infty(r)$. In the isotropic approximation the displacement field must satisfy Navier's equation, eqn.(4.4), which in the absence of body forces becomes:

$$\mu\nabla^2\mathbf{u}^\infty + (\lambda+\mu)\nabla(\nabla\cdot\mathbf{u}^\infty) = 0.$$

Exercise 5.1 By using sphercial polar coordinates show that the general purely radial solution of Navier's equation is:

$$u_r(r) = Ar + D/r^2 \tag{5.1}$$

with $u_\theta = u_\phi = 0$. A and D are arbitrary constants. ■

Since $\mathbf{u}^\infty$ must be finite at $r = \infty$ we choose $u^\infty(r) = D/r^2$. The constant D is determined by the boundary condition at the surface of the hole: $u^\infty(r_h) = r_s - r_h$. Therefore $D = (r_s - r_h)r_h^2$.

One of the surprising features of this model is that the dilation is zero everywhere. Inside the sphere there is no elastic strain because the sphere is assumed to be rigid. Outside the sphere the strain in the radial direction is $e_{rr} = \mathrm{d}u_r^\infty/\mathrm{d}r = -2D/r^2$, while $e_{\theta\theta} = e_{\phi\phi} = u_r/r = D/r^2$, so that the trace of the strain tensor is zero. But there is an overall volume change ΔV^∞ and it is all located in the misfitting sphere: $\Delta V^\infty = (4\pi/3)(r_s^3 - r_h^3) \approx 4\pi r_h^2(r_s - r_h) = 4\pi D$.

[2] B. A. Bilby, Proc. Phys. Soc. A **63**, 191 (1950)
[3] Bruce A. Bilby FRS (1922-2013)

Exercise 5.2 The strain tensor in spherical coordinates is as follows:

$$
\begin{aligned}
e_{rr} &= \frac{\partial u_r}{\partial r} \\
e_{\theta\theta} &= \frac{1}{r}\frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r} \\
e_{\phi\phi} &= \frac{1}{r\sin\theta}\frac{\partial u_\phi}{\partial \phi} + \frac{u_r}{r} + u_\theta \frac{\cot\theta}{r} \\
e_{r\phi} &= \frac{1}{2}\left(\frac{1}{r\sin\theta}\frac{\partial u_r}{\partial \phi} - \frac{u_\phi}{r} + \frac{\partial u_\phi}{\partial r}\right) \\
e_{r\theta} &= \frac{1}{2}\left(\frac{1}{r}\frac{\partial u_r}{\partial \theta} - \frac{u_\theta}{r} + \frac{\partial u_\theta}{\partial r}\right) \\
e_{\phi\theta} &= \frac{1}{2}\left(\frac{1}{r}\frac{\partial u_\phi}{\partial \theta} - \frac{u_\phi \cot\theta}{r} + \frac{1}{r\sin\theta}\frac{\partial u_\theta}{\partial \phi}\right)
\end{aligned}
$$

Hence explain both mathematically and geometrically why $e_{\theta\theta} = e_{\phi\phi} = u_r/r$ for a displacement field that is purely radial.

■

In reality all bodies are finite. Consider a finite body with a free surface $\mathscr{S}$. The solution for the misfitting sphere in an infinite medium has to be corrected by applying surface tractions $-\sigma^\infty_{ij} n_j$ over the surface $\mathscr{S}$, where $\sigma^\infty_{ij} = 2\mu\partial u^\infty_i/\partial x_j$, and in Cartesian coordinates $u^\infty_i = Dx_i/r^3$. These tractions cancel those that would exist on the surface if the infinite solution were not corrected. To calculate the change ΔV^I in the volume of the body caused by this distribution of surface tractions consider the integral:

$$
\int_{\mathscr{S}} \sigma^\infty_{ij} x_i n_j \mathrm{d}S = \int_V (\sigma^\infty_{ij} x_i)_{,j} \mathrm{d}V = \int_V \sigma^\infty_{ij,j} x_i + \sigma^\infty_{ij}\delta_{ij} \mathrm{d}V = \int_V -f_i x_i \mathrm{d}V + V\langle\sigma_{ii}\rangle,
$$

where the divergence theorem and the equilibrium condition have been used. Since there is no body force in V the average trace of the stress tensor is $\langle\sigma_{ii}\rangle$ inside the body when the distribution of surface tractions $-\sigma^\infty_{ij} n_j$ is applied is given by:

$$
\begin{aligned}
\langle\sigma_{ii}\rangle &= -\int_{\mathscr{S}} \sigma^\infty_{ij} x_i n_j \mathrm{d}S \\
&= -\int_{\mathscr{S}} 2\mu D\left(\frac{\delta_{ij}}{r^3} - \frac{3x_i x_j}{r^5}\right) x_i n_j \mathrm{d}S \\
&= 4\mu D \int_{\mathscr{S}} \frac{x_i n_i}{r^3} \mathrm{d}S,
\end{aligned}
$$

where $(x_i n_i/r^3)\mathrm{d}S$ is an element of solid angle, and the final surface integral is therefore 4π. The change in volume, ΔV^I, caused by the elimination of the surface tractions is given by $3B\Delta V^I = \langle\sigma_{ii}\rangle = 16\pi\mu D = 4\mu\Delta V^\infty$. The total volume change caused by the misfitting sphere in a finite body

is given by:

$$\Delta V = \Delta V^{\infty} + \Delta V^{I} = 4\pi D\left(\frac{3B+4\mu}{3B}\right) = 3\Delta V^{\infty}\left(\frac{1-\nu}{1+\nu}\right), \tag{5.2}$$

where we have used $B = 2\mu(1+\nu)/(3(1-2\nu))$, and ν is Poisson's ratio. For $\nu = 1/3$, which is typical of many metals, the increase in the overall volume of the body as a result of the presence of free surfaces is approximately 50%. It is remarkable that this result does not depend on the size of the body, or its shape, or where the defect is located within it. This is an example of an insight from a simple model into a universal property of point defects that would be virtually impossible to obtain from a purely atomistic model.

Exercise 5.3 Consider a misfitting *non*-rigid sphere at the centre of a much larger sphere of radius R on the surface of which there are no tractions. The radius of the hole into which the misfitting sphere is inserted is r_h. The radius of the unconstrained (i.e. stress-free) non-rigid sphere is r_s. The bulk modulus and the shear modulus of the large sphere of radius R are B and μ respectively, and the bulk modulus of the misfitting sphere is B'.

Show that the volume change of the sphere of radius R is

$$\Delta V = \left(\frac{1+\frac{4\mu}{3B}}{1+\frac{4\mu}{3B'}}\right)\delta v$$

where $\delta v = 4\pi r_h^2(r_s - r_h)$ is the misfit volume.

Show that the dilation in the large sphere is

$$e_{ii} = \frac{\frac{4\mu}{3B}}{1+\frac{4\mu}{3B'}}\frac{\delta v}{V},$$

where $V = 4\pi R^3/3$ is the volume of the sphere of radius R.

■

5.3 Interaction energies

The misfitting sphere model has been used widely owing to its attractive simplicity. But its central assumption that the defect has spherical symmetry limits its applicability principally to substitutional defects at sites of cubic symmetry. It is less applicable to interstitial defects which may display highly non-spherical symmetries, such as split interstitials and crowdion defects. We saw in section 4.5 how the multipole expansion may be applied to derive the displacement field of a substitutional point defect. It may also be applied to the displacement field of an interstitial defect, with the sole difference that the defect forces are the entire forces, rather than the excess forces, exerted by the foreign atom on the surrounding neighbours in the equilibrium state. The multipole expansion captures the symmetry of the site occupied by the defect. In this section we consider the interaction energy between two point defects using the multipole expansion. This is a hybrid approach using interatomic forces to describe the sources of the elastic fields and elasticity theory to describe the interactions over distances much larger than the atomic scale. The analysis of this section follows Siems (1968) [4].

We begin by thinking about the problem entirely from an atomistic viewpoint. In eqn.(3.28) we wrote down the harmonic expansion of the potential energy of the crystal. Here we write it slightly

[4] R. Siems Phys. Stat. Sol. **30**, 645-658 (1968)

differently:

$$E = -\sum_n f_i^{(n)} u_i^{(n)} + \frac{1}{2}\sum_n \sum_p \frac{\partial^2 E}{\partial u_i^{(n)} \partial u_j^{(p)}} u_i^{(n)} u_j^{(p)}, \tag{5.3}$$

where we interpret the forces $f_i^{(n)}$ as being forces due to an existing defect which create the displacement field $u_i^{(n)}$. Let the vector of defect forces be $\mathbf{f}$, the vector of atomic displacements be $\mathbf{u}$ and the matrix of second derivatives be $\mathbf{S}$. Then we can rewrite eqn.(5.3) for the potential energy of the defect as follows:

$$E = -\mathbf{f}\cdot\mathbf{u} + \frac{1}{2}\mathbf{uSu} = -\frac{1}{2}\mathbf{f}\cdot\mathbf{u} = -\frac{1}{2}\mathbf{uSu},$$

where E is minimised when $\mathbf{f} = \mathbf{Su}$. Notice that this energy is negative. It is the energy of *relaxing* the system of defect forces and harmonic atomic interactions. The defect forces do work when the atoms on which they act are displaced thereby reducing the potential energy by $-\mathbf{f}\cdot\mathbf{u}$. These displacements induce further displacements that extend throughout the crystal and which raise the potential energy by $\frac{1}{2}\mathbf{uSu}$. A balance between these two competing terms is established when $\mathbf{f} = \mathbf{Su}$, and the reduction in the potential energy is then only half of $-\mathbf{f}\cdot\mathbf{u}$.

If there is a second defect, with defect force vector $\tilde{\mathbf{f}}$ and vector of atomic displacements $\tilde{\mathbf{u}}$, with $\tilde{\mathbf{f}} = \mathbf{S}\tilde{\mathbf{u}}$ and $\tilde{E} = -\frac{1}{2}\tilde{\mathbf{f}}\cdot\tilde{\mathbf{u}}$, we may use the linear superposition principle to write the total potential energy as follows:

$$\begin{aligned} E^T &= -(\mathbf{f}+\tilde{\mathbf{f}})\cdot(\mathbf{u}+\tilde{\mathbf{u}}) + \frac{1}{2}(\mathbf{u}+\tilde{\mathbf{u}})\mathbf{S}(\mathbf{u}+\tilde{\mathbf{u}}) \\ &= E + \tilde{E} + E_{int} \end{aligned}$$

where the interaction energy E_{int} is given by:

$$\begin{aligned} E_{int} &= -(\mathbf{f}\cdot\tilde{\mathbf{u}} + \tilde{\mathbf{f}}\cdot\mathbf{u}) + \frac{1}{2}(\mathbf{uS\tilde{u}} + \tilde{\mathbf{u}}\mathbf{Su}) \\ &= -\mathbf{f}\cdot\tilde{\mathbf{u}} = -\tilde{\mathbf{f}}\cdot\mathbf{u}. \end{aligned} \tag{5.4}$$

The last equality follows from Maxwell's reciprocity theorem. This result for the interaction energy may be understood in the following way. Suppose the first defect already exists and we introduce the second defect. The atoms on which the defect forces $\mathbf{f}$ of the first defect act are displaced further by the displacement field $\tilde{\mathbf{u}}$ of the second defect. The additional work done is $-\mathbf{f}\cdot\tilde{\mathbf{u}}$. If we repeat the argument but with the second defect existing before the first the work done is $-\tilde{\mathbf{f}}\cdot\mathbf{u}$.

To describe the interaction energy over large separations between the defects we may use defect forces from an atomistic calculation and elasticity theory to evaluate the displacement field. That is why we call this a hybrid approach.

With the first point defect at the origin of the Cartesian coordinate system the interaction energy with a second point defect at $\mathbf{x}$ is

$$E_{int} = -\sum_n \tilde{f}_i(\mathbf{R}^{(n)}) u_i(\mathbf{x}+\mathbf{R}^{(n)}) \tag{5.5}$$

where $\tilde{f}_i(\mathbf{R}^{(n)})$ is the force exerted by the defect at $\mathbf{x}$ on its neighbour at the relative position $\mathbf{R}^{(n)}$ and $u_i(\mathbf{x}+\mathbf{R}^{(n)})$ is the displacement of this neighbour due to the defect at the origin. Provided $|\mathbf{x}| \gg |\mathbf{R}^{(n)}|$ we may expand $u_i(\mathbf{x}+\mathbf{R}^{(n)})$ about $u_i(\mathbf{x})$:

$$u_i(\mathbf{x}+\mathbf{R}^{(n)}) = u_i(\mathbf{x}) + R^{(n)}_j u_{i,j}(\mathbf{x}) + \frac{1}{2} R^{(n)}_j R^{(n)}_k u_{i,jk}(\mathbf{x}) + \frac{1}{6} R^{(n)}_j R^{(n)}_k R^{(n)}_l u_{i,jkl}(\mathbf{x}) + \dots \tag{5.6}$$

Substituting this Taylor expansion into the interaction energy, eqn.(5.5), we obtain:

$$E_{int} = -\cancel{\left(\sum_n \tilde{f}_i(\mathbf{R}^{(n)}) \right)} u_i(\mathbf{x}) - \tilde{\rho}_{ij} u_{i,j}(\mathbf{x}) - \frac{1}{2} \tilde{q}_{ijk} u_{i,jk}(\mathbf{x}) - \frac{1}{6} \tilde{o}_{ijkl} u_{i,jkl}(\mathbf{x}) - \dots \tag{5.7}$$

where the sum of the defect forces is zero provided the defect at $\mathbf{x}$ is relaxed, and $\tilde{\rho}_{ij}$, $\tilde{q}_{ijk}$ and $\tilde{o}_{ijkl}$ are the dipole, quadrupole and octopole moments respectively of the forces exerted by the defect at $\mathbf{x}$.

We can now use the multipole expansion, eqn.(4.21), to expand the displacement field due to the defect at the origin:

$$\begin{aligned} u_i(\mathbf{x}) &= \sum_m G_{ia}(\mathbf{x}-\mathbf{R}^{(m)}) f_a(\mathbf{R}^{(m)}) \\ &= \sum_m \left(G_{ia}(\mathbf{x}) - R^{(m)}_b G_{ia,b}(\mathbf{x}) + \frac{1}{2} R^{(m)}_b R^{(m)}_c G_{ia,bc}(\mathbf{x}) - \frac{1}{6} R^{(m)}_b R^{(m)}_c R^{(m)}_d G_{ia,bcd}(\mathbf{x}) + \dots \right) f_a(\mathbf{R}^{(m)}) \\ &= G_{ia}(\mathbf{x}) \cancel{\sum_m f_a(\mathbf{R}^{(m)})} - G_{ia,b}(\mathbf{x}) \rho_{ab} + \frac{1}{2} G_{ia,bc}(\mathbf{x}) q_{abc} - \frac{1}{6} G_{ia,bcd}(\mathbf{x}) o_{abcd} + \dots \end{aligned} \tag{5.8}$$

The sum of the forces exerted by the defect at the origin on its neighbours is zero provided the defect is relaxed. The dipole, quadrupole and octopole moments of the forces exerted by the defect at the origin are ρ_{ab}, q_{abc}, o_{abcd} respectively. Inserting the displacement field $u_i(\mathbf{x})$ into the interaction energy of eqn.(5.7), and collecting terms involving the same order of differentiation of the Green's function we obtain finally:

$$\begin{aligned} E_{int} &= \tilde{\rho}_{ij} G_{ia,bj}(\mathbf{x}) \rho_{ab} \\ &+ \frac{1}{2} \left(\tilde{q}_{ijk} G_{ia,bjk}(\mathbf{x}) \rho_{ab} - \tilde{\rho}_{ij} G_{ia,bcj}(\mathbf{x}) q_{abc} \right) \\ &+ \frac{1}{12} \left(2\tilde{o}_{ijkl} G_{ia,bjkl}(\mathbf{x}) \rho_{ab} + 2\tilde{\rho}_{ij} G_{ia,bcdj}(\mathbf{x}) o_{abcd} - 3\tilde{q}_{ijk} G_{ia,bcjk}(\mathbf{x}) q_{abc} \right) + \dots \end{aligned} \tag{5.9}$$

The first line is the dipole-dipole interactions and it decays as $1/|\mathbf{x}|^3$. The second line is the dipole-quadrupole interaction and it decays as $1/|\mathbf{x}|^4$. The third line describes interactions that depend on the fourth derivative of the Green's function, which decays as $1/|\mathbf{x}|^5$, and involves quadrupole-quadrupole interactions and dipole-octopole interactions.

Exercise 5.4 Consider two point defects in an elastically isotropic infinite crystal occupying sites of cubic symmetry. Aligning the coordinate axes with the sides of the cube show that the dipole tensor is $\rho_{ij} = p\delta_{ij}$.

Hence show that the dipole-dipole interaction energy is zero.

Show that the quadrupole tensor is zero (*hint* the elements of the quadrupole tensor q_{ijk} transform under a rotation in the same way as $x_i x_j x_k$).

Show that there are only two non-zero independent elements of the octopole tensor: o_{1111}

and $o_{1122} = o_{1212} = o_{1221}$. Hence show that the octopole tensor may be expressed as:

$$o_{ijkl} = o_{1111}\delta_{ijkl} + o_{1122}\left(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - 3\delta_{ijkl}\right).$$

where $\delta_{ijkl} = 1$ if $i = j = k = l$, zero otherwise.

Show that the first non-zero term in the interaction energy between the defects is:

$$E_{int} = \frac{1}{6}G_{ij,jiii}\left[p(\tilde{o}_{1111} - 3\tilde{o}_{1122}) + \tilde{p}(o_{1111} - 3o_{1122})\right] + \frac{1}{2}G_{ij,jikk}(p\tilde{o}_{1122} + \tilde{p}o_{1122}),$$

where $G_{ij,jiii}$ means $G_{1j,j111} + G_{2j,j222} + G_{3j,j333}$.

Hence show that

$$E_{int} = \frac{7(1-2\nu)}{16\pi\mu(1-\nu)x^5}\left[p(\tilde{o}_{1111} - 3\tilde{o}_{1122}) + \tilde{p}(o_{1111} - 3o_{1122})\right]\left(\frac{5(x_1^4 + x_2^4 + x_3^4)}{x^4} - 3\right)$$

Thus, in an infinite isotropic cubic crystal like tungsten two vacancies interact through the dipole-octopole interaction.

■

5.4 The λ-tensor

In the previous section we saw that a point defect at **x** has an interaction energy with another elastic field according to eqn.(5.7). Thus, if the strain field with which it interacts is homogeneous then the interaction energy involves only the dipole tensor, a strain gradient at **x** will interact with the quadrupole tensor, the second derivative of the strain at **x** will interact with the octopole tensor of the defect, and so on. If there is a dilute solution of these point defects their dipole tensors can drive a change of shape of the crystal. If c is the atomic concentration of the point defect then the λ-tensor describes the rate of change of the spontaneous homogeneous strain of the crystal with c in the absence of any forces applied to the surface of the crystal:

$$\lambda_{kl} = \frac{\mathrm{d}e^h_{kl}}{\mathrm{d}c} \tag{5.10}$$

To expose the relationship between the λ-tensor and the dipole tensor consider the elastic energy of the crystal containing a solution of the defects. It is assumed that the defects are sufficiently far apart that their defect forces do not overlap, and therefore the dipole tensors are the same as those for an isolated defect. In a volume V let there be N defects. If the atomic volume of the host atoms is Ω then $c = N\Omega/V$ in the dilute limit. If the crystal undergoes a homogeneous strain e^h_{ij} the elastic energy of the volume V becomes:

$$E = -N\rho_{ij}e^h_{ij} + \frac{V}{2}c_{ijkl}e^h_{ij}e^h_{kl}.$$

Minimising this elastic energy with respect to the homogeneous strain we obtain:

$$N\rho_{ij} = Vc_{ijkl}e^h_{kl}$$

Substituting $N = Vc/\Omega$ and differentiating the resulting expression with respect to the concentration c we obtain:

$$\rho_{ij} = \Omega c_{ijkl}\lambda_{kl} \tag{5.11}$$

This is a very useful relationship because the λ-tensor is experimentally measurable using X-ray diffraction for example.

5.5 Problem set 5

1. Consider two point defects occupying sites of cubic point group symmetry in a slightly anisotropic cubic crystal, such as aluminium for which the anisotropy ratio is 1.2. Their elastic dipole tensors are $\tilde{\rho}_{ij} = \tilde{d}\delta_{ij}$ and $\rho_{ij} = \delta_{ij}d$. The elastic interaction energy at large separations is given by:

$$E_{int} = \tilde{\rho}_{ij}G_{ia,jb}(\mathbf{x})\rho_{ab} = \tilde{d}dG_{ij,ji}(\mathbf{x}).$$

We have seen in Exercise 5.4 that in an elastically isotropic medium $G_{ij,ji} = 0$. Using eqn.(4.43) for the first order correction to the Fourier transform of the elastic Green's function in a cubic crystal show that

$$\begin{aligned} G_{ij,ji}(\mathbf{x}) &= -\left(\frac{c_{11}-c_{12}-2c_{44}}{(c_{12}+2c_{44})^2}\right)\frac{1}{(2\pi)^3}\int\frac{k_1^4+k_2^4+k_3^4}{k^4}e^{-i\mathbf{k}\cdot\mathbf{x}}\mathrm{d}^3k \\ &= -\left(\frac{3}{8\pi}\right)\left(\frac{c_{11}-c_{12}-2c_{44}}{(c_{12}+2c_{44})^2}\right)\frac{1}{x^3}\left[5\frac{x_1^4+x_2^4+x_3^4}{x^4}-3\right] \end{aligned} \tag{5.12}$$

We recognise the same angular dependence[5] in this interaction energy as was found in Exercise 5.4 for the dipole-octopole interaction between two point defects in an isotropic medium. However, the dipole-dipole interaction energy in a cubic crystal varies with separation x as $1/x^3$, as compared with $1/x^5$ for the variation of the dipole-octopole interaction energy in an isotropic crystal. Therefore, whenever there is a significant departure of the anisotropy ratio from unity in a cubic crystal the dipole-dipole interaction will always dominate at long-range.

2. Consider a substitutional point defect located at the origin of a Cartesian coordinate system in an infinite simple cubic crystal structure with lattice constant a. The forces exerted by the defect on each of the six nearest neighbours have magnitude f, and they are directed along the bonds. Show that the displacement field $u_i(\mathbf{x})$ at $\mathbf{x}$ is approximately $-2afG_{ij,j}(\mathbf{x})$, and state the nature of the approximation.

Show that in the isotropic elastic approximation:

$$u_i(\mathbf{x}) = \frac{(1-2\nu)af}{4\pi\mu(1-\nu)}\frac{x_i}{x^3}.$$

Hence calculate the volume change ΔV^∞ associated with the point defect in an infinite medium. By comparing your answer with ΔV^∞ in the model of a point defect as a misfitting

[5]The angular dependence is the cubic harmonic $K_{4,1} = (\sqrt{21}/4)[5((x_1/x)^4 + (x_2/x)^4 + (x_3/x)^4) - 3]$, which is normalised as follows: $\int (K_{4,1})^2 \mathrm{d}\Omega = 4\pi$ where $\mathrm{d}\Omega = \sin\theta \mathrm{d}\theta\mathrm{d}\phi$ is an element of solid angle. Cubic harmonics are combinations of spherical harmonics with cubic symmetry. See W. R. Fehlner and S. H. Vosko, Can. J. Phys. **54**, 2159-2169 (1976).

sphere in an infinite medium obtain an expression for $D = \Delta V^{\infty}/(4\pi)$ in the misfitting sphere model in terms of the bond length a and defect force f.

6. Dislocations

6.1 Introduction

When crystals are deformed there is a limit to which the deformation remains elastic or reversible. Beyond this limit the crystal fractures if it is brittle. If it is ductile further deformation takes place, but the additional deformation is irreversible or 'plastic'. When the load is removed from a ductile crystal that has been deformed plastically the shape of the crystal has changed permanently. It is a characteristic property of many metals and alloys that they can undergo plastic deformation before they fracture, which enables them to be extruded, pressed, rolled and forged into everyday objects from car bodies to drink cans and furniture to girders for bridges and skyscrapers.

In the early twentieth century there was a great deal of interest to discover what happened inside a crystal when it ceased to deform elastically and began to deform plastically. It was a mystery why some crystals such as copper and gold were extremely ductile whereas others such as diamond were brittle, at least at room temperature. Equally baffling was the observation that some body centred cubic metals that were ductile at room temperature became brittle at low temperatures displaying almost no ductility before they fractured, while some face centred cubic metals remained ductile at temperatures as low as a few degrees Kelvin. The rate at which a crystal was deformed was also found to have a strong influence on the ductile/brittle behaviour of many crystalline materials. The purity of the crystal was also found to affect the stress required to make it deform plastically. Beginning to address these questions brought about the birth of the science of materials in the 1930s. With the advent of transmission electron microscopy in the 1950s it was possible to see what was happening inside very thin crystals undergoing plastic deformation. Today our understanding of all these phenomena and processes is based on dislocations and how they interact with other defects in the material. But the complexity of many phenomena is so great that our understanding is still far from complete, and we shall return to some of these issues in Chapter 10.

6.2 Dislocations as the agents of plastic deformation

To a very good approximation crystals deform plastically at constant volume. Permanent changes of shape are brought about by shearing processes in which planes of atoms slide over each other.

The sliding creates steps at the surface of the crystal, which creates surface roughness that can be felt with a finger if a metal paperclip is straightened. In 1926 Frenkel[1] produced a startling back-of-an-envelope calculation demonstrating that the stress required to slide a plane of atoms en masse over another was orders of magnitude larger than the stresses observed to initiate plastic deformation of many metals.

Consider two adjacent planes of atoms in a crystal spaced d apart. Let the crystal periodicity in the plane in the direction of sliding be b. Frenkel sought to calculate the maximum stress required to slide one entire plane rigidly over the other. Let x be the relative displacement of the two atomic planes in the direction of sliding. Let $\gamma(x)$ be the energy per unit area of the plane associated with this relative displacement. What do we know about $\gamma(x)$? We know it must be periodic, with a period of b, and that $\gamma(x)$ is minimised when $x = nb$ where n in an integer. Therefore we can write

$$\gamma(x) = A_0 + \sum_{n=1}^{\infty} A_n \cos\frac{2n\pi x}{b} + B_n \sin\frac{2n\pi x}{b}, \tag{6.1}$$

which is just a Fourier expansion of $\gamma(x)$. If we make the simplest approximation and assume $\gamma(x)$ is an even function, taking just the first term of the cosine series we obtain $\gamma(x) = A\sin^2(\pi x/b)$, where A is a constant with the dimensions of energy per unit area. The slope of $\gamma(x)$ is the negative of the stress required to sustain the relative displacement x. Frenkel argued that as $x \to 0$ this slope is determined by the elastic shear modulus μ because $\mathrm{d}\gamma/\mathrm{d}x = (A\pi/b)\sin(2\pi x/b) \to A2\pi^2 x/b^2$ and this has to be equated to $\mu x/d$. Therefore, $A = (\mu b^2)/(2\pi^2 d)$ and the stress required to slide one plane of atoms rigidly and en masse over another is of order $\mu b/(2\pi d)$.

The stress required to transition from elastic to plastic deformation is called the yield stress. Frenkel's estimate of the yield stress is of order $\mu/10$. Experimentally observed values of the yield stress are typically between 3 and 5 orders of magnitude less than this. We have to conclude that entire planes of atoms do not slide en masse over each other during plastic deformation.

The resolution of this paradox came with the independent but almost simultaneous insights of Orowan[2] in Budapest, Polanyi in Manchester (UK) [3] and Taylor[4] in Cambridge (UK) in 1934 who suggested that planes 'slip' past each other through the movement of linear defects called dislocations separating slipped and unslipped regions. Taylor's paper is especially remarkable as it includes a detailed discussion of the crystallographic nature of slip, namely the observation that it occurs on particular planes in particular directions, and of the hardening of crystals that occurs with increasing plastic deformation, which is called work hardening, and elastic interactions between dislocations leading to stable and unstable configurations of dislocations. Taylor drew on the earlier mathematical treatment of dislocations by Volterra[5] who was interested in the elastic equilibrium of bodies rendered multiply connected through the existence of dislocations[6].

The sliding of one crystal plane over another, which is called slip, begins with the nucleation of a small dislocation loop. The plane where slip occurs is called the slip plane. Inside the loop the planes have slipped past each other by a vector **b**, which is called the Burgers vector. Outside the loop the planes have not slipped. The dislocation is the line separating the slipped and unslipped regions of the slip plane - see Fig.6.1. We will show that under the influence of an applied shear stress on the slip plane in the direction of **b** the loop expands converting more of the unslipped

[1] Jacov Frenkel (1894-1952), Soviet condensed matter physicist.

[2] Egon Orowan FRS (1902 -1989) in Z. Physik **89**, 634. https://doi.org/10.1007/BF01341480

[3] Michael Polanyi FRS (1891-1976) in Z. Physik **89**, 660. https://doi.org/10.1007/BF01341481

[4] Sir Geoffrey Ingram Taylor FRS, OM (1891-1976) in Proc. Roy. Soc. A **145**, 388. https://doi.org/10.1098/rspa.1934.0106

[5] Vito Volterra, Italian mathematician and physicist (1860-1940)

[6] V. Volterra, Annales scientifiques de l'École Normale Supérieure (1907) **24** 401-517, (1907). http://archive.numdam.org/article/ASENS_1907_3_24__401_0.pdf

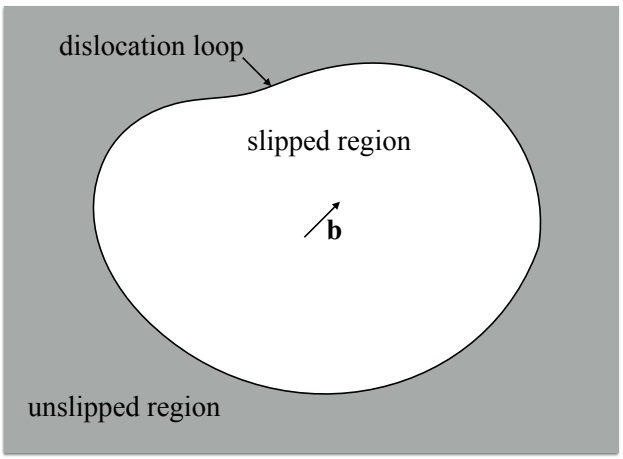

Figure 6.1: A dislocation loop lying in a slip plane separating slipped and unslipped regions. The dislocation is the line separating the slipped and unslipped regions of the slip plane. Inside the loop the material beneath the slip plane has been translated with respect to material above it by the Burgers vector **b**.

region into slipped region and enabling the applied shear stress to do more work thereby reducing the potential energy of the whole system, which includes an external loading mechanism if there is one. If the loop is in a single crystal then when it reaches the surfaces of the crystal the entire crystal on one side of the slip plane has slipped by **b** with respect to the other side, and there is a step on the surface with unit normal $\hat{\mathbf{n}}$ of height $(\mathbf{b}\cdot\hat{\mathbf{n}})$. If the Burgers vector **b** is a crystal lattice vector in the slip plane then as the dislocation moves it recreates the same crystal structure in its wake. In principle **b** may be any lattice vector in the slip plane, but we shall see that the elastic energy of the dislocation varies as $|\mathbf{b}|^2$ so that usually only the smallest lattice vectors are found. The smallest lattice vectors tend to occur in planes with the largest spacing.

The key physical insight of Orowan, Polanyi and Taylor in 1934 is that slip by dislocation motion localises the inevitable bond breaking and making, when one plane slides over another, to the very much smaller region where the dislocation line is located. In contrast when an entire plane slides en masse over another the bond breaking and making occurs everywhere in the slip plane simultaneously. Therefore, the stress required to move a dislocation is orders of magnitude less than that required to slide a plane of a macroscopic crystal over another en masse. This was a giant step forward. But fundamental questions remained, such as why some crystals seem to undergo very limited slip, if any, before they fracture, why some are brittle at low temperatures and ductile at higher temperatures, why small concentration of impurities can have a seemingly disproportionate effect on the ease of slip, the choice of slip plane and Burgers vector, the stress to move a dislocation, how dislocations are created, and even whether they do in fact exist. Answering these questions over the intervening years has led to some of the most interesting experimental, theoretical and computational condensed matter physics, which continues to have profound consequences for engineering and technology.

6.3 Characterisation of dislocations: the Burgers circuit

Consider a dislocation loop lying in a slip plane. Within the loop there is a constant relative displacement of the crystals above and below the slip plane equal to the Burgers vector. Because the relative displacement is constant throughout the slipped region inside the loop it does not vary with the direction of the dislocation line. Where the direction of the dislocation line is perpendicular to the Burgers vector the dislocation is said to have 'edge' character. Perhaps the reason for this name is that the dislocation line is then along the edge of a terminating half-plane, as shown in Fig.6.2. An edge dislocation is a long straight dislocation where the dislocation line is everywhere

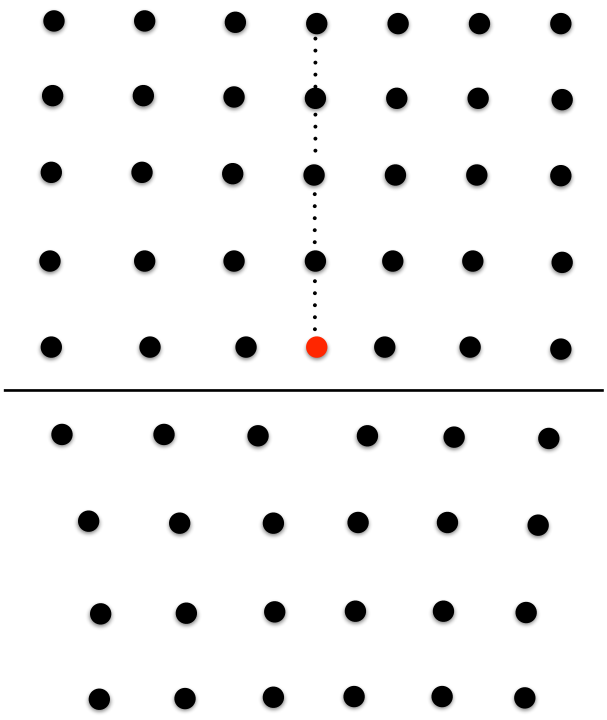

Figure 6.2: A schematic illustration of an edge dislocation viewed along the dislocation line. Each dot represent a column of atoms normal to the page. The horizontal line is the trace of the slip plane. Above the slip plane there is an extra half plane shown by dotted lines. The edge dislocation is located at the termination of this extra half plane, which is shown by the column of atoms in red.

perpendicular to the Burgers vector. The edge dislocation appeared in Taylor's paper of 1934. When the dislocation line is parallel to the Burgers vector the dislocation is said to have 'screw' character. A screw dislocation is a long straight dislocation where the dislocation line is everywhere

parallel to the Burgers vector. The screw dislocation was introduced by J M Burgers[7] in 1939[8]. The reason for this name is that the crystal lattice planes normal to the dislocation line become a helicoidal surface like the thread of a screw, as shown in Fig.6.3. If the angle between the line direction and the Burgers vector is ϕ then the dislocation may be regarded as a superposition of an edge dislocation with Burgers vector $\mathbf{b}\sin\phi$ and a screw dislocation with Burgers vector $\mathbf{b}\cos\phi$. Such a dislocation is said to have 'mixed' character, and its atomic structure changes from screw to edge type as ϕ varies from 0 to $\pi/2$.

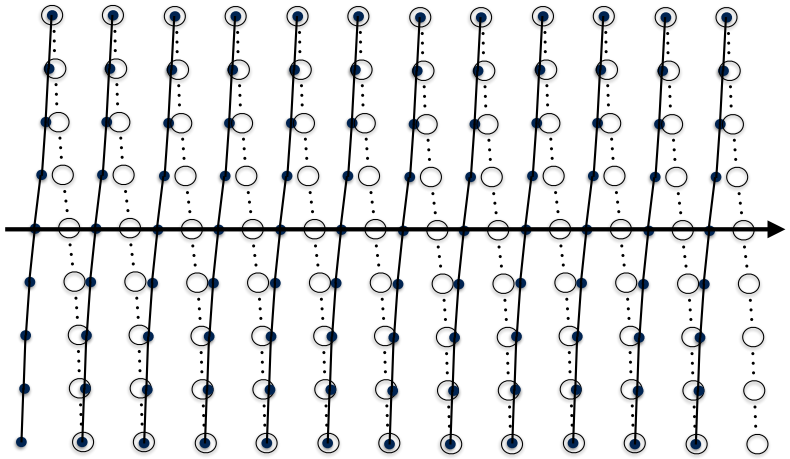

Figure 6.3: A schematic illustration of a screw dislocation. The dislocation line is shown by the horizontal arrow. Solid circles and solid lines are below the page. Open circles and dotted lines are above the page. Planes of atoms are converted into a continuous spiral by the dislocation. This drawing was adapted from D. Hull and D. J. Bacon, *Introduction to Dislocations*, Pergamon Press: Oxford, 3rd edn. (1984).

Suppose we see some defect in a crystal. How do we know whether it is a dislocation or some other defect? If it is a dislocation how do we determine its Burgers vector? The answer to both questions is the Burgers circuit construction. This is a geometrical construction that was introduced by Frank[9] in a paper which defined rigorously many of the terms in use today when discussing dislocations and plasticity of crystals[10]. The construction is illustrated in Fig.6.4 for an edge dislocation. We draw a closed circuit in the elastically distorted crystal surrounding the dislocation which begins and ends at the same site. The circuit comprises steps between lattice sites

[7] Johannes Martinus Burgers (1895-1981), whose brother, Wilhelm Gerard Burgers (1897-1988), also worked on dislocations.

[8] J. M. Burgers, Koninklijke Nederlandsche Akademie van Wetenschappen, **42**, 293 (1939), available online at `http://www.dwc.knaw.nl/toegangen/digital-library-knaw/?pagetype=publDetail&pId=PU00014649`

[9] Sir Charles Frank FRS (1911-1998)

[10] F. C. Frank, Phil. Mag. **42**, 809 (1951), available online at `http://dx.doi.org/10.1080/14786445108561310`

of the elastically distorted crystal. It is important that the circuit passes through material that is recognisable as perfect crystal that has only been elastically strained, and that it does not go near the core of the dislocation where the local atomic environment cannot be mapped onto the perfect crystal. It does not matter how far the circuit goes from the dislocation as long as it does not enclose any other dislocations and as long as it keeps away from the dislocation core. The circuit is then mapped onto a perfect lattice, as shown in Fig.6.4. If the defect is a dislocation the circuit mapped

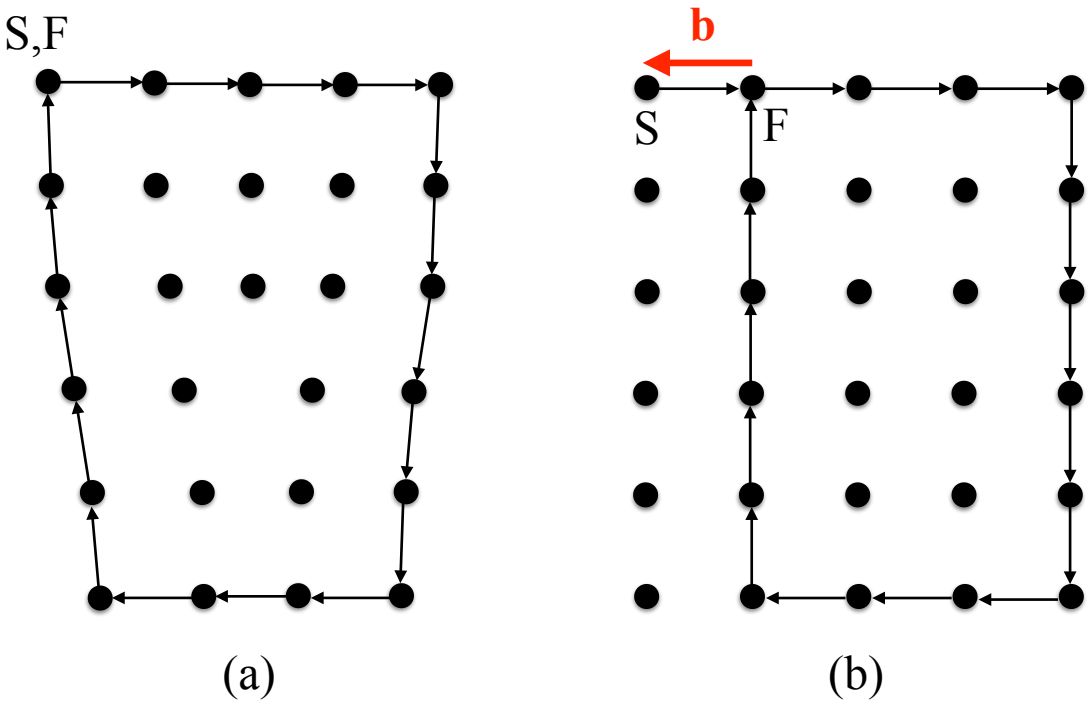

Figure 6.4: Illustration of the Burgers circuit construction for an edge dislocation. The line sense of the edge dislocation in (a) is defined to be positive looking into the page. A right handed circuit is drawn around the dislocation line, starting at S and finishing at the same site F. The circuit is mapped, step by step, onto the perfect crystal in (b). It is found that S and F are no longer coincident, and therefore the circuit has a closure failure. The vector joining F to S, shown in red, is defined by the FS/RH convention as the Burgers vector **b** of the dislocation.

onto the perfect lattice will not close. By convention, the closure failure from the finish to the start of the circuit mapped onto the perfect crystal is the Burgers vector when the circuit is taken in a clockwise sense when looking along the dislocation line. But if the circuit is started somewhere else or follows a different closed path in the dislocated crystal the Burgers vector will always be the same provided the circuit does not enclose any other dislocations and that it does not pass through the dislocation core. The Burgers vector is an invariant property of the dislocation. The existence of the closure failure when the circuit is mapped into the perfect crystal is the defining property of

a dislocation[11]. There is no closure failure if the circuit encloses a point defect only.

A bit more terminology: when the Burgers vector is a lattice vector the dislocation is said to be a'perfect' dislocation. When the Burgers vector is a fraction of a lattice vector the dislocation is called a 'partial' dislocation.

6.4 Glide, climb and cross-slip

When dislocations move in their slip plane no diffusion of atoms is required. This kind of motion is called *glide* or conservative because the number of atoms at the dislocation as it moves along is conserved. The normal to the slip plane of an edge dislocation is $\hat{\mathbf{n}} = \hat{\mathbf{b}} \times \hat{\mathbf{t}}$, where $\hat{\mathbf{b}}$ is a unit vector parallel to the Burgers vector and $\hat{\mathbf{t}}$ is a unit vector along the line direction. As long as an edge dislocation moves within its slip plane the number of atoms in the extra half-plane associated with the dislocation does not change, and this is why such motion is conservative.

If an edge dislocation moves out of its slip plane then the extra half plane either grows or shrinks requiring atoms to be added or removed from it. This is called *climb* or non-conservative motion. Because diffusion is involved the speed of climb is generally much less than the speed of glide. Climb may enable an edge dislocation to overcome an obstacle blocking glide on its slip plane, but since diffusion is involved this is a thermally activated process. The extra half plane of an edge dislocation grows when atoms are added to it, which is equivalent to saying that vacancies are emitted from it. In this way edge dislocations are sources and sinks for vacancies and self-interstitials, and thus they can regulate the populations of these point defects when the populations deviate from those in thermal equilibrium, e.g. due to irradiation.

In contrast to an edge dislocation the slip plane of a screw dislocation is not uniquely defined because $\mathbf{b}$ and $\hat{\mathbf{t}}$ are parallel or anti-parallel to each other. Consequently a screw dislocation gliding on one plane may switch to gliding on another plane, which is a process called cross-slip. For example, a screw dislocation in a body-centred cubic (b.c.c.) crystal with Burgers vector $\mathbf{b} = 1/2[111]$ gliding on a $(1\bar{1}0)$ plane may cross-slip onto the planes $(10\bar{1})$ or $(0\bar{1}1)$. As a result screw dislocations move only conservatively. Cross-slip provides a mechanism for screw dislocations to overcome barriers to glide on a slip plane by gliding on an inclined plane over or under the obstacle. Although cross-slip is a process that happens during glide it is thermally activated. In face-centred cubic (f.c.c.) crystals this is because perfect dislocations may be dissociated into partial dislocations separated by stacking faults (see the next chapter), and before cross-slip can take place the partial dislocations have to be recombined which is a process requiring energy. But even when perfect dislocations cross-slip the atomic structure of the dislocation core has to adjust from that on one slip plane to that on another, and this is also a process requiring energy.

Exercise 6.1 During irradiation with high energy neutrons a highly non-equilibrium population of vacancies is created in a metal. In a b.c.c. crystal some of the vacancies cluster together on a $\{111\}$-type plane forming hexagonal dislocation loops with sides along $\langle 1\bar{1}0 \rangle$ directions. The Burgers vector of the dislocation loop is $1/2\langle 111 \rangle$ type. Show that such a loop may move in a conservative manner in the direction of its Burgers vector, tracing out a hexagonal prism as it moves. Such a loop is called 'prismatic' for this reason. This example illustrates how individual defects, vacancies in this case, may come together to form a new defect, a prismatic dislocation loop in this case, and the mechanism of their motion changes from diffusion of individual vacancies to glide of the loop as a whole involving no diffusion at all. ■

[11] The Burgers circuit is an example of anholonomy which arises elsewhere in physics including the Aharonov-Bohm effect, Foucault's pendulum and the Berry phase.

6.5 The interaction energy between a dislocation and another source of stress

This section and the following section are based on the analysis presented in section 5 of a review paper by Eshelby[12]. Consider a dislocation D in a body with external surface S_o. There may be constant tractions acting on the surface of the body, and other defects D′ inside the body creating internal stresses. Define a closed surface S inside the body enclosing D only so that it separates D from other sources of internal stress and the external load. The position of S is otherwise arbitrary. The internal surface S divides the body into two regions: region I contains D and region II is the rest of the body, as illustrated in Fig.6.5.

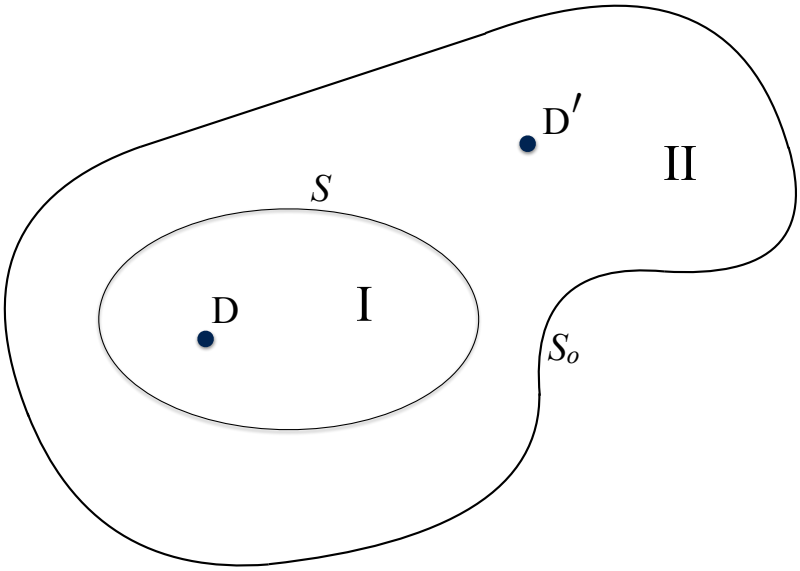

Figure 6.5: A schematic illustration of a body with an external surface S_o containing a dislocation D and other defects represented by D′. The internal closed surface S separates D from the other defects in the body, and divides the body into region I containing D only and region II which is the remainder of the body.

Let the elastic fields created by D be u_i^D, e_{ij}^D and σ_{ij}^D. Let u_i^A, e_{ij}^A and σ_{ij}^A be the elastic fields created by the constant loads applied to the external surface and by sources of internal stress other than D. Using linear superposition the total elastic fields in the body are $\sigma_{ij} = \sigma_{ij}^D + \sigma_{ij}^A$, $e_{ij} = e_{ij}^D + e_{ij}^A$ and $u_i = u_i^D + u_i^A$. The total elastic energy density is $\frac{1}{2}\sigma_{ij}e_{ij} = \frac{1}{2}(\sigma_{ij}^D + \sigma_{ij}^A)(e_{ij}^D + e_{ij}^A)$. The elastic interaction energy density involves only the cross terms between D and A, so that the total interaction energy is the following integral:

$$E_{int} = \frac{1}{2}\int_V \left(\sigma_{ij}^D e_{ij}^A + \sigma_{ij}^A e_{ij}^D\right)\, \mathrm{d}V. \tag{6.2}$$

[12] J. D. Eshelby, in *Solid State Physics*, 3 (1956), pp.79-144. Reprinted in *Collected Works of J. D Eshelby*, eds. X. Markenscoff and A. Gupta, Springer: Dordrecht, The Netherlands, (2006), pp. 143-208.

In region I u_i^D cannot be defined everywhere owing to the elastic singularity D, but u_i^A is well defined throughout region I. Similarly u_i^A cannot be defined everywhere in region II, but u_i^D is well defined throughout region II. It follows from Hooke's law that $\sigma_{ij}^A e_{ij}^D = \sigma_{ij}^D e_{ij}^A$. Therefore eqn.6.2 can be rewritten as:

$$E_{int} = \int_I \sigma_{ij}^D u_{i,j}^A \, \mathrm{d}V + \int_{II} \sigma_{ij}^A u_{i,j}^D \, \mathrm{d}V. \tag{6.3}$$

Furthermore, $\sigma_{ij,j}^D = 0$ and $\sigma_{ij,j}^A = 0$ in the absence of body forces and therefore $\sigma_{ij}^D u_{i,j}^A = (\sigma_{ij}^D u_i^A)_{,j}$ and $\sigma_{ij}^A u_{i,j}^D = (\sigma_{ij}^A u_i^D)_{,j}$. The divergence theorem then transforms eqn.6.3 into the following surface integrals:

$$E_{int} = \int_S \sigma_{ij}^D u_i^A \, n_j \mathrm{d}S + \int_{S_0} \sigma_{ij}^A u_i^D \, n_j \, \mathrm{d}S - \int_S \sigma_{ij}^A u_i^D \, n_j \, \mathrm{d}S. \tag{6.4}$$

If there is no external loading mechanism then the external surface is free and $\sigma_{ij}^A n_j = 0$. The integral over S_0 then vanishes. But if there is a load applied to the surface S_0 of the body then the potential energy of the loading mechanism must be included in the interaction energy. The potential energy of the external loading mechanism may be equated to:

$$E_{ext} = -\int_{S_0} \sigma_{ij}^A u_i^D n_j \mathrm{d}S, \tag{6.5}$$

because if D moves then the displacement field u_i^D will change by δu_i^D and the external load will do work given by $\int_{S_0} \sigma_{ij}^A \, \delta u_i^D \mathrm{d}S$. The potential energy of the loading mechanism will then change by $-\int_{S_0} \sigma_{ij}^A \, \delta u_i^D \mathrm{d}S$. Thus the total interaction energy, including the potential energy of the loading mechanism, is as follows:

$$E_{int}^T = E_{int} + E_{ext} = \int_S \left(\sigma_{ij}^D u_i^A - \sigma_{ij}^A u_i^D \right) n_j \, \mathrm{d}S. \tag{6.6}$$

Thus, the integral over the external surface of the body in eqn.6.4 vanishes in the total interaction energy irrespective of whether there is an external load applied to the body or not.

If D is a dislocation loop enclosing a surface Σ then Σ may be taken as the cut on either side of which the displacement by the Burgers vector **b** exists. Then the surface S may be taken as the positive and negative sides of Σ together with a tube of around the dislocation line, as shown in Fig.6.6. As the radius of the tube shrinks to zero it contributes nothing to the integral in eqn.6.6. The first term in the integral in eqn.6.6 varies continuously on crossing Σ, and therefore contibutes nothing. But there is a discontinuity in the displacement u_i^D on either side of the cut equal to b_i. Therefore the total interaction energy becomes:

$$E_{int}^T = -b_i \int_{\Sigma^+} \sigma_{ij}^A n_j \, \mathrm{d}S, \tag{6.7}$$

This equation has a clear physical interpretation. If we imagine the dislocation loop is created in the presence of the stress field σ_{ij}^A then E_{int}^T represents the work done by the stress field σ_{ij}^A when the two sides of Σ undergo the relative displacement by the Burgers vector.

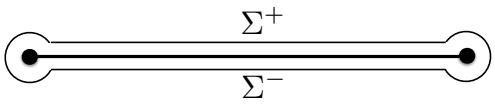

Figure 6.6: Illustration of the surface of the integral in eqn.6.6 for a dislocation loop. The loop is viewed edge on and the plane of the loop is the thicker horizontal line. The dislocation line is normal to the page and is represented by the black circles at the ends of the plane of the loop. The surface S comprises the surfaces Σ^+ and Σ^- above and below the plane of the loop and a tube surrounding the dislocation.

Exercise 6.2 Using Maxwell's reciprocity theorem (eqn.4.7) show that the interaction energy between two dislocation loops A and B is as follows:

$$E_{int} = -b_i^A \int_{\Sigma_A} \sigma_{ij}^B n_j \, \mathrm{d}S = -b_i^B \int_{\Sigma_B} \sigma_{ij}^A n_j \, \mathrm{d}S. \tag{6.8}$$

■

6.6 The Peach-Koehler force on a dislocation

Now that we have the interaction energy in eqn.6.7 we may derive a general expression for the force on a dislocation due to an applied stress field. This force was first derived[13] by Peach and Koehler[14] and it is known as the Peach-Koehler force.

Consider a dislocation where the local direction of the dislocation line is $\hat{\mathbf{t}}$. Suppose an infinitesimal segment $\mathrm{d}l$ of the dislocation line is displaced by a vector $\mathrm{d}\mathbf{s}$, as shown in Fig.6.7. The vector area swept by the displaced segment is $\mathrm{d}\mathbf{A} = \mathrm{d}l\hat{\mathbf{t}} \times \mathrm{d}\mathbf{s}$. As in the previous section let σ_{ij}^A be the stress field acting locally on the dislocation segment, where this stress is the resultant of the stresses due to an external loading mechanism and sources of internal stresses. The displacement of the dislocation segment changes the surface Σ in the surface integral of eqn.6.7. The change in the energy of interaction between the dislocation and the applied stress is given by the change of

[13] M O Peach and J S Koehler, Phys. Rev. **80**, 436 (1950), available online at `https://journals.aps.org/pr/pdf/10.1103/PhysRev.80.436`.

[14] This work formed part of the doctoral thesis of M O Peach under the supervision of James Stark Koehler (1914-2006) undertaken at Carnegie Institute of Technology.

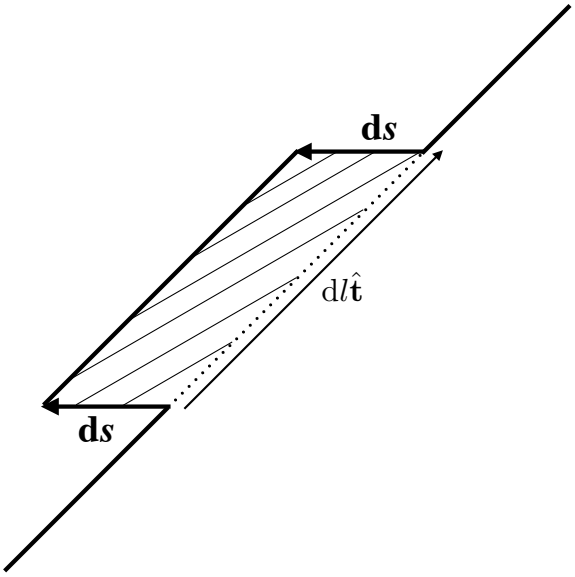

Figure 6.7: A segment of dislocation of length dl moves by the vector d$\mathbf{s}$ sweeping the area shaded.

E^T_{int} in eqn.6.7:

$$\mathrm{d}E^T_{int} = -b_i\,\sigma^A_{ij}\,\mathrm{d}l\,\varepsilon_{jpq}\,t_p\,\mathrm{d}s_q \tag{6.9}$$

The force acting on the dislocation segment is $-\partial E^T_{int}/\partial s_q = F_q\,\mathrm{d}l$, where F_q is the force per unit length:

$$F_q = b_i\,\sigma^A_{ij}\,\varepsilon_{jpq}t_p = \varepsilon_{qjp}\left(\sigma^A_{ji}\,b_i\right)t_p. \tag{6.10}$$

In vector notation this is $\mathbf{F} = (\boldsymbol{\sigma}\mathbf{b}) \times \hat{\mathbf{t}}$. This is the Peach-Koehler force. The force is always perpendicular to the dislocation line. For edge dislocations, where the slip plane is uniquely defined, it includes components that promote glide and climb of dislocations. If $\hat{\mathbf{n}}$ is the normal to the slip plane the climb component is $\mathbf{F}_c = (\mathbf{F}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}$ and the glide component is $\mathbf{F}_g = \mathbf{F} - \mathbf{F}_c = \hat{\mathbf{n}} \times (\mathbf{F} \times \hat{\mathbf{n}})$.

Exercise 6.3 Show that the glide component of the Peach-Koehler force per unit length on any dislocation is τb where τ is the shear stress resolved on the slip plane in the direction of the Burgers vector and b is the magnitude of the Burgers vector.

Show that the climb component of the Peach-Koehler force on an edge dislocation is σb where σ is the resolved normal stress in the direction of the Burgers vector. ■

6.7 Volterra's formula

We come now to the derivation of a general expression for the displacement field of a dislocation loop in anisotropic elasticity. This expression is useful because, as shown[15] by Nabarro[16], the displacement field for an infinitesimal loop may be integrated to obtain solutions for loops of arbitrary shapes and sizes, which may then be differentiated to give strain fields and stress fields using Hooke's law. Assign an arbitrary line sense to the dislocation loop. Looking along the positive direction of the dislocation line draw a right-handed circuit around the dislocation line. The positive and negatives sides of the cut are above and below the dislocation line on this circuit. The third line of eqn.4.12 gives the displacement field in an infinite medium when displacements are prescribed on a surface $\mathscr{S}$. We may use this relation to write down the displacement field of a dislocation loop $\mathscr{L}$ with a displacement discontinuity equal to the Burgers vector between the positive and negative sides of a cut surface $\mathscr{S}$ bounded by $\mathscr{L}$. The result is known as Volterra's formula:

$$u_j(\mathbf{x}) = -c_{mikp}\, b_k \int_{\mathscr{S}^+} G_{ij,m'}(\mathbf{x}-\mathbf{x}')\, n_{p'} \mathrm{d}S' = c_{mikp}\, b_k \int_{\mathscr{S}^+} G_{ij,m}(\mathbf{x}-\mathbf{x}')\, n_{p'} \mathrm{d}S', \tag{6.11}$$

where the integration is carried out on the positive side $\mathscr{S}^+$ of the cut only.

A dislocation loop created in this way is called a Volterra dislocation. It is a mathematical simplification of a real dislocation in the sense that it is a mathematical line where the displacement discontinuity equal to the Burgers vector appears infinitely abruptly. In other words a Volterra dislocation has no width, and the displacement by the Burgers vector appears as a step function at the dislocation line. Real dislocations in crystals have finite widths, which are called dislocation cores, where the relative displacement by the Burgers vector accumulates over several interatomic bond lengths. Nevertheless the concept of a Volterra dislocation describes the elastic field away from the core quite accurately. In the next chapter we will meet more realistic models of dislocations.

The stress and strain fields of the loop are more significant physically than the displacement field because they determine the energy of the loop and its interaction with other defects. In contrast to the stress and strain fields of the loop, the displacement field is inevitably dependent on the choice of the cut where the displacement by the Burgers vector is introduced. Differentiation of the displacement field obtained with Volterra's formula yields the strain field, which must be independent of the cut. Later in this chapter we will derive Mura's formula for the *strain* field of the dislocation which depends only on the configuration of the dislocation *line*, and not on the cut bounded by it.

6.8 The infinitesimal loop

Consider a loop of infinitesimal area δA and unit normal n_p located at $\mathbf{x}'$. Volterra's formula, eqn.6.11, provides the displacement field at $\mathbf{x}$:

$$\delta u_j(\mathbf{x}) = \delta A\, c_{mikp}\, b_k\, n_p\, G_{ij,m}(\mathbf{x}-\mathbf{x}'). \tag{6.12}$$

This expression is exact within linear anisotropic elasticity. If the loop is finite, with a characteristic size L, then it remains a good approximation provided $|\mathbf{x}-\mathbf{x}'|$ is more than about 2L. To see that this is true consider a finite, planar, centrosymmetric loop, with its centre located at $\mathbf{R}$, where we

[15] F. R. N. Nabarro, Phil. Mag. **42**, 1224 (1951), available online at `http://dx.doi.org/10.1080/14786444108561379`

[16] Frank Nabarro FRS (1916-2006)

take the cut to be the plane of area A bounded by the loop. Writing $\mathbf{x}' = \mathbf{R} + \boldsymbol{\rho}$ we have the Taylor expansion:

$$G_{ij,m}(\mathbf{x}-\mathbf{R}-\boldsymbol{\rho}) = G_{ij,m}(\mathbf{x}-\mathbf{R}) - \rho_p\, G_{ij,mp}(\mathbf{x}-\mathbf{R}) + \frac{1}{2}\rho_p\,\rho_q\, G_{ij,mpq}(\mathbf{x}-\mathbf{R}) - \ldots$$

Inserting this into Volterra's formula, eqn.6.11, we obtain an expansion for the displacement field of the loop in terms of its areal moments:

$$u_j(\mathbf{x}) = c_{mikp}\, b_k\, n_p \left[G_{ij,m}(\mathbf{x}-\mathbf{R})A - G_{ij,mp}(\mathbf{x}-\mathbf{R}) \int_S \rho_p \,\mathrm{d}S + \frac{1}{2}\, G_{ij,mpq}(\mathbf{x}-\mathbf{R}) \int_S \rho_p\,\rho_q \,\mathrm{d}S - \ldots \right] \tag{6.13}$$

For a centrosymmetric loop, such as a circle, ellipse, rectangle, hexagon etc., only the even moments are non-zero. The first correction to eqn.6.12 comes from second moments of the form $G_{ij,mpp}(\mathbf{x}-\mathbf{R}) \int_S \rho_p^2 \mathrm{d}S$, which is of order $L^4/|\mathbf{x}-\mathbf{R}|^4$. Thus, provided the distance from a finite centrosymmetric loop is more than about twice its size eqn.6.12 is remarkably accurate.

In isotropic elasticity eqn.6.12 becomes:

$$\delta u_j(\mathbf{x}) = -\frac{\delta A\, b_k\, n_p}{8\pi(1-\nu)} \left[(1-2\nu)\frac{\delta_{kj}X_p + \delta_{pj}X_k - \delta_{kp}X_j}{X^3} + 3\frac{X_k X_p X_j}{X^5} \right], \tag{6.14}$$

where $\mathbf{X} = \mathbf{x} - \mathbf{x}'$. By integrating this expression the displacement fields of finite loops may be derived in isotropic elasticity. The displacement fields of infinite straight dislocations may be found by considering loops closed at infinity.

6.9 The dipole tensor of an infinitesimal loop

The leading term in the interaction energy between two point defects in the multipole expansion of eqn.5.9 involves their dipole tensors. Since an infinitesimal dislocation loop is also a point defect it should be possible to define a dipole tensor for it too. One way to derive the dipole tensor for an infinitesimal loop is to consider the interaction energy between two infinitesimal loops A and B using eqn.6.8. If loop A is at the origin and loop B is at $\mathbf{x}$ then the interaction energy between them is as follows:

$$\delta E_{int} = -b_f^B n_g^B (\delta A^B)(\delta \sigma_{fg}^A(\mathbf{x})), \tag{6.15}$$

where δA^B is the area of loop B, and $\delta\sigma_{fg}^A(\mathbf{x})$ is the stress field of the infinitesimal loop A located at the origin evaluated at loop B. Taking only the first term of the moment expansion of the displacement field of a loop in eqn.6.13, and differentiating it to obtain the strain field we obtain:

$$\delta\sigma_{fg}^A(\mathbf{x}) = c_{fgjl} c_{mikp} b_k^A n_p^A (\delta A^A) G_{ij,ml}(\mathbf{x}). \tag{6.16}$$

Inserting this stress field into eqn.6.15 we obtain an expression for the elastic interaction energy in terms of the dipole tensors $\delta\rho$ of the infinitesimal loops:

$$\delta E_{int} = -\delta\rho_{jl}^B G_{ij,ml}(\mathbf{x}) \delta\rho_{mi}^A, \tag{6.17}$$

where

$$\begin{aligned}\delta\rho^A_{mi} &= c_{mikp}b^A_k n^A_p(\delta A^A)\\ \delta\rho^B_{jl} &= c_{jlfg}b^B_f n^B_g(\delta A^B).\end{aligned} \tag{6.18}$$

As with the interaction energy between two point defects eqn.6.17 separates properties of the loops themselves contained in the dipole tensors from the radial and angular dependences of their interaction energy contained in the second derivatives of the Green's function. The dipole tensor of a loop in eqn.6.18 has a simple physical interpretation. As first discussed[17] by Kroupa[18] a dislocation loop may be thought of as a region that has undergone a transformation strain $e^T_{kp} = \frac{1}{2}(b_k n_p + b_p n_k)/\Delta$ where Δ is the thickness of the transformed region in the direction of the loop normal. (We will take the limit $\Delta \to 0$.) The transformation strain gives rise to a stress $\sigma^T_{im} = c_{imkp}e^T_{kp} = c_{imkp}b_k n_p/\Delta$. The surfaces of the loop are separated by the vector $\hat{\mathbf{n}}\Delta$. These surfaces are subjected to equal and opposite forces per unit area equal to $\sigma^T_{im}n_m$. The displacement at $\mathbf{x}$ is then given by:

$$u_j(\mathbf{x}) = \int_{S'} G_{ji}(\mathbf{x}-\mathbf{x}')\sigma^T_{im}n_m \mathrm{d}S',$$

where the integration is over the surface of the transformed region constituting the loop. Inside the loop σ^T_{im} is constant. Applying the divergence theorem we obtain:

$$u_j(\mathbf{x}) = \sigma^T_{im}\int_{V'} G_{ji,m}(\mathbf{x}-\mathbf{x}')\mathrm{d}V',$$

where the integral is over the volume of the transformed region. In the limit of an infinitesimal loop, and in the limit of $\Delta \to 0$, the volume integral becomes $G_{ji,m}(\mathbf{x})(\delta A)\Delta$ where δA is the area of the loop with normal $\hat{\mathbf{n}}$. The displacement field of the infinitesimal loop is therefore as follows:

$$u_j(\mathbf{x}) = c_{imkp}\frac{b_k n_p}{\Delta}\Delta(\delta A)G_{ji,m}(\mathbf{x}) = c_{imkp}b_k n_p(\delta A)G_{ji,m}(\mathbf{x}) = \rho_{im}G_{ji,m}(\mathbf{x}). \tag{6.19}$$

As discussed by Landau and Lifshitz[19] and the paper[20] by Burridge and Knopoff[21] the displacement by the Burgers vector at a dislocation may be thought of as the response of the medium to a dipolar distribution of fictitious forces across the cut. These forces are fictitious in the sense that they are the forces required by linear elasticity to generate the displacement by the Burgers vector. They are equivalent to Kanzaki forces in harmonic lattice theory, which are the forces required to create a defect within a harmonic model of atomic interactions. The real forces are what we have called 'defect forces', and they are the true forces acting between atoms, as determined by quantum mechanics. But in a linear elastic theory it is the fictitious forces we need to generate a dislocation and they appear in the dipole tensor for the dislocation loop.

[17] F. Kroupa in *Theory of crystal defects*, Proceedings of the Summer School held in Hrazany in September 1964, Academia Publishing House of the Czechoslovak Academy of Sciences (1966), pp 275-316

[18] František Kroupa (1925-2009)

[19] L. D Landau and E. M. Lifshitz, *Theory of Elasticity*, Pergamon Press: Oxford, 3rd edition (1986), section 27, p.111

[20] R. Burridge and L. Knopoff, Bulletin of the Seismological Society of America **54**, 1875-1888 (1964), available online at: `http://bssa.geoscienceworld.org/content/ssabull/54/6A/1875.full.pdf`

[21] Leon Knopoff (1925-2011) geophysicist, member of the NAS

6.10 Mura's formula

We have already noted that the displacement field of a dislocation depends on the choice of the cut across which the relative displacement by the Burgers vector is introduced. This is explicit in Volterra's formula, eqn.6.11. However, the strain and stress fields cannot depend on the choice of cut. Nevertheless, we can differentiate Volterra's formula to get the distortion field:

$$u_{j,g}(\mathbf{x}) = c_{mikp} b_k \int_{\mathscr{S}^+} G_{ij,mg}(\mathbf{x}-\mathbf{x}') n_{p'} \mathrm{d}S', \tag{6.20}$$

but this also involves an integral over the cut surface. The distortion field should be independent of the choice of the cut and dependent only on the configuration of the dislocation line. Mura's formula makes this explicit by transforming the surface integral in eqn.6.20 into a line integral along the dislocation line using a version of Stokes' theorem.

A familiar form of Stokes' theorem is:

$$\int_S \varepsilon_{ijk} V_{k,j'}(\mathbf{x}-\mathbf{x}') n'_i \mathrm{d}S(\mathbf{x}') = \oint_L V_p(\mathbf{x}-\mathbf{x}') \, \mathrm{d}x_{p'}, \tag{6.21}$$

where L is the closed line where the surface S terminates. In this equation $\mathbf{x}$ is constant and $\mathbf{x}'$ ranges over the surface S and around the line L. In the following we revert to our usual notation $\mathrm{d}S(\mathbf{x}') = \mathrm{d}S'$. To obtain the version of Stokes' theorem needed here let $V_k(\mathbf{x}-\mathbf{x}') = f(\mathbf{x}-\mathbf{x}')\delta_{kq}$ so that the vector function $\mathbf{V}(\mathbf{x}-\mathbf{x}')$ has only one non-zero component and that is $V_q(\mathbf{x}-\mathbf{x}') = f(\mathbf{x}-\mathbf{x}')$. Then Stokes' theorem becomes:

$$\varepsilon_{qij} \int_S f_{,j'}(\mathbf{x}-\mathbf{x}') n'_i \mathrm{d}S' = \oint_L f(\mathbf{x}-\mathbf{x}') \, \mathrm{d}x'_q.$$

Multiplying both sides of this equation by ε_{qpg} we obtain the desired form:

$$\begin{aligned}
\varepsilon_{qpg}\varepsilon_{qij} \int_S f_{,j'}(\mathbf{x}-\mathbf{x}') n'_i \mathrm{d}S' &= \varepsilon_{qpg} \oint_L f(\mathbf{x}-\mathbf{x}') \, \mathrm{d}x'_q \\
(\delta_{ip}\delta_{jg} - \delta_{jp}\delta_{ig}) \int_S f_{,j'}(\mathbf{x}-\mathbf{x}') n'_i \mathrm{d}S' &= \varepsilon_{qpg} \oint_L f(\mathbf{x}-\mathbf{x}') \, \mathrm{d}x'_q \\
\int_S f_{,g'}(\mathbf{x}-\mathbf{x}') n'_p \mathrm{d}S' &= \int_S f_{,p'}(\mathbf{x}-\mathbf{x}') n'_g \mathrm{d}S' + \varepsilon_{qpg} \oint_L f(\mathbf{x}-\mathbf{x}') \, \mathrm{d}x'_q
\end{aligned} \tag{6.22}$$

If we set $f(\mathbf{x}-\mathbf{x}') = G_{ij,m'}(\mathbf{x}-\mathbf{x}')$ then we obtain:

$$\int_S G_{ij,m'g'}(\mathbf{x}-\mathbf{x}') n'_p \mathrm{d}S' = \int_S G_{ij,m'p'}(\mathbf{x}-\mathbf{x}') n'_g \mathrm{d}S' + \varepsilon_{qpg} \oint_L G_{ij,m'}(\mathbf{x}-\mathbf{x}') \, \mathrm{d}x'_q. \tag{6.23}$$

Multiplying both sides by c_{mikp} we obtain:

$$c_{mikp} \int_S G_{ij,m'g'}(\mathbf{x}-\mathbf{x}') n'_p \mathrm{d}S' = c_{mikp} \int_S G_{ij,m'p'}(\mathbf{x}-\mathbf{x}') n'_g \mathrm{d}S' + c_{mikp}\varepsilon_{qpg} \oint_L G_{ij,m'}(\mathbf{x}-\mathbf{x}') \, \mathrm{d}x'_q. \tag{6.24}$$

Recalling that $G_{ij,m'p'} = G_{ij,mp}$, it follows from the defining equation, (eqn.4.8), for the Green's function that $c_{mikp}G_{ij,m'p'} = 0$ at all points except $\mathbf{x}' = \mathbf{x}$. Since the surface S can always be chosen

to avoid $\mathbf{x}$ the surface integral on the right hand side is zero. Inserting this result in eqn.6.20 we obtain Mura's formula for the distortion tensor:

$$u_{j,g}(\mathbf{x}) = \varepsilon_{qpg}\, c_{mikp} b_k \oint_{L'} G_{ij,m'}(\mathbf{x}-\mathbf{x}')\, \mathrm{d}x_{q'}, \tag{6.25}$$

The stress field of the dislocation follows from Hooke's law: $\sigma_{ab}(\mathbf{x}) = c_{abjg} u_{j,g}(\mathbf{x})$. In isotropic elasticity this becomes:

$$\sigma_{ab}(\mathbf{x}) = c_{abjg} \frac{\varepsilon_{qpg} b_k}{8\pi(1-\nu)} \oint_{L'} \left[(1-2\nu) \frac{\delta_{kj}X_p + \delta_{pj}X_k - \delta_{kp}X_j}{X^3} + 3\frac{X_k X_p X_j}{X^5} \right] \mathrm{d}x_{q'},$$

where $\mathbf{X} = \mathbf{x} - \mathbf{x}'$. Defining the line integral I_{kjpq} as

$$I_{kjpq} = \oint_{L'} \left[(1-2\nu) \frac{\delta_{kj}X_p + \delta_{pj}X_k - \delta_{kp}X_j}{X^3} + 3\frac{X_k X_p X_j}{X^5} \right] \mathrm{d}x_{q'}$$

the stress field may be conveniently expressed as follows:

$$\sigma_{ab}(\mathbf{x}) = \frac{\mu b_k}{8\pi(1-\nu)} \left[\frac{2\nu}{1-2\nu} \delta_{ab} \varepsilon_{qpj} I_{kjpq} + \varepsilon_{qpb} I_{kapq} + \varepsilon_{qpa} I_{kbpq} \right]. \tag{6.26}$$

6.11 The stress field of an edge dislocation in isotropic elasticity

To illustrate the application of Mura's formula the stress field of an infinitely long edge dislocation along the x_3-axis with $\mathbf{b} = [b,0,0]$ will be derived. In eqn.6.26 we have $b_k = b\delta_{k1}$ and $q = 3$. We obtain:

$$\begin{aligned}
\sigma_{11} &= \frac{\mu b}{4\pi(1-\nu)(1-2\nu)} \left(\nu I_{1213} - (1-\nu) I_{1123}\right) \\
\sigma_{12} &= \sigma_{21} = \frac{\mu b}{8\pi(1-\nu)} \left(I_{1113} - I_{1223}\right) \\
\sigma_{13} &= \sigma_{31} = -\frac{\mu b}{8\pi(1-\nu)} I_{1323} \\
\sigma_{22} &= \frac{\mu b}{4\pi(1-\nu)(1-2\nu)} \left((1-\nu) I_{1213} - \nu I_{1123}\right) \\
\sigma_{23} &= \sigma_{32} = \frac{\mu b}{8\pi(1-\nu)} I_{1313} \\
\sigma_{33} &= \frac{\mu b}{4\pi(1-\nu)(1-2\nu)} \nu (I_{1213} - I_{1123}) = \nu\left(\sigma_{11} + \sigma_{22}\right).
\end{aligned}$$

It is straightforward to evaluate the integrals:

$$
\begin{aligned}
I_{1213} &= -\frac{2(1-2\nu)x_2}{\left(x_1^2+x_2^2\right)}+\frac{4x_1^2x_2}{\left(x_1^2+x_2^2\right)^2} \\
I_{1123} &= \frac{2(1-2\nu)x_2}{\left(x_1^2+x_2^2\right)}+\frac{4x_1^2x_2}{\left(x_1^2+x_2^2\right)^2} \\
I_{1113} &= \frac{2(1-2\nu)x_1}{\left(x_1^2+x_2^2\right)}+\frac{4x_1^3}{\left(x_1^2+x_2^2\right)^2} \\
I_{1223} &= \frac{2(1-2\nu)x_1}{\left(x_1^2+x_2^2\right)}+\frac{4x_1x_2^2}{\left(x_1^2+x_2^2\right)^2} \\
I_{1313} &= I_{1323}=0
\end{aligned}
$$

We obtain the following stress components for an edge dislocation in isotropic elasticity:

$$
\begin{aligned}
\sigma_{11} &= -\frac{\mu b}{2\pi(1-\nu)}x_2\frac{3x_1^2+x_2^2}{\left(x_1^2+x_2^2\right)^2} \\
\sigma_{12} &= \frac{\mu b}{2\pi(1-\nu)}x_1\frac{x_1^2-x_2^2}{\left(x_1^2+x_2^2\right)^2} \\
\sigma_{13} &= 0 \\
\sigma_{22} &= \frac{\mu b}{2\pi(1-\nu)}x_2\frac{x_1^2-x_2^2}{\left(x_1^2+x_2^2\right)^2} \\
\sigma_{23} &= 0 \\
\sigma_{33} &= -\frac{\mu b\nu}{\pi(1-\nu)}\frac{x_2}{\left(x_1^2+x_2^2\right)}
\end{aligned}
\tag{6.27}
$$

We see in eqn.6.27 that the stress field is inversely proportional to the distance from the dislocation line. This is a general feature of straight dislocations. In particular the stress diverges as the dislocation line is approached. This follows from the assumption that the dislocation is a mathematical line with no width. In more realistic models the dislocation has a finite width and the stress does not become infinite.

Exercise 6.4 Sketch the stress components of eqn.6.27 in the x_1-x_2 plane. Sketch the hydrostatic stress $\frac{1}{3}\mathrm{Tr}\,\sigma$ for the edge dislocation. Edge dislocations attract misfitting atoms. Where would a larger misfitting atom tend to locate itself to lower its elastic misfit energy?

■

6.12 The elastic energy of a dislocation

The elastic energy of a dislocation is just the volume integral of the elastic energy density it creates:

$$E_{el}=\frac{1}{2}\int_V \sigma_{ij}u_{i,j}\mathrm{d}V.$$

It would be quite laborious to evaluate the elastic energy in this way as there are usually many non-zero stress and strain components. However, the task can be simplified significantly by applying the divergence theorem.

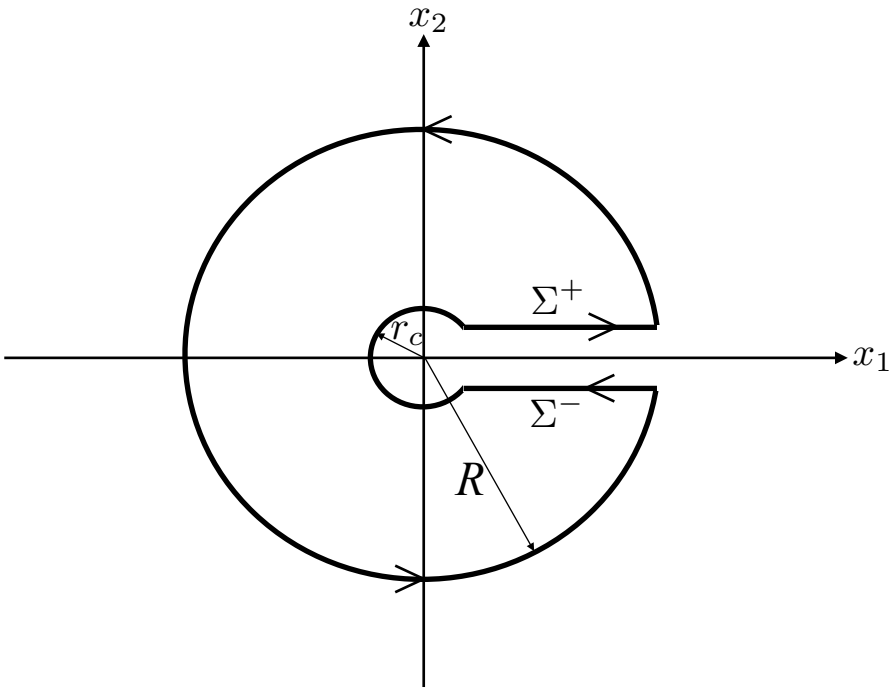

Figure 6.8: To illustrate the evaluation of the surface integral in eqn.6.28 for a straight dislocation lying along the x_3-axis. The positive line sense of the dislocation is coming out of the page. A right-handed circuit C is therefore anti-clockwise, as shown by the arrows.

Consider an infinite straight dislocation parallel to the x_3-axis in an anisotropic elastic medium. Let the cut surface coincide with the half-plane $x_2 = 0$ where $x_1 \geq 0$, as shown in Fig.6.8. Applying the divergence theorem to the elastic strain energy per unit length along x_3, and recalling that $\sigma_{ij,j} = 0$, we obtain:

$$E_{el} = \frac{1}{2}\int_C \sigma_{ij}\, u_i\, n_j \,\mathrm{d}S, \tag{6.28}$$

where the surface C comprises four segments of until length along x_3. The first is the almost complete small cylinder of radius r_c around the dislocation line. In the limit the separation of the surfaces on either of the cut becomes infinitesimal the cylinder of radius r_c becomes complete. The integral of $\sigma_{ij}n_j$ around the cylinder is then zero because there is no resultant force associated with the dislocation line. The same argument applies to the segment around the outer cylinder of radius

R, and it too is zero. That leaves the two contributions from the segments Σ^+ and Σ^- on either side of the cut. As the separation of the segments shrinks to zero they become:

$$E_{el} = \frac{1}{2}\int_{r_c}^{R} \sigma_{i2}(x_1,0)\, b_i \,\mathrm{d}x_1 \tag{6.29}$$

For example, for an edge dislocation $b_i = b\delta_{i1}$, and the only stress component contributing to this integral is $\sigma_{12}(x_1,0)$. Thus we obtain the following energy per unit length of an edge dislocation in isotropic elasticity:

$$E_{el}^{edge} = \frac{1}{2}\int_{r_c}^{R} \frac{\mu b^2}{2\pi(1-\nu)}\frac{\mathrm{d}x_1}{x_1} = \frac{\mu b^2}{4\pi(1-\nu)}\ln(R/r_c). \tag{6.30}$$

For a screw dislocation $b_i = b\delta_{i3}$, and the only stress component contributing to the integral in eqn.6.29 is $\sigma_{32}(x_1,0)$. In the isotropic elastic approximation the energy per unit length of a screw dislocation is as follows:

$$E_{el}^{screw} = \frac{\mu b^2}{4\pi}\ln(R/r_c) \tag{6.31}$$

The logarithmic divergence of the energy of a straight dislocation is common to other line singularities in physics, e.g. the electrostatic energy per unit length of an infinitely long thin line of charge, or the magnetic energy per unit length of an infinitely long thin wire carrying a constant current. Of course dislocations exist in crystals of finite size, so their energy never becomes infinite. More significantly, dislocations often lower their elastic energies by organising themselves into configurations where their elastic fields have much shorter spatial extent than they would have if each dislocation were isolated. A classic example of such screening is the elastic field of a grain boundary comprising an array of dislocations with a spacing d. It is found (see the Problems at the end of this chapter) that the elastic field decays exponentially from the grain boundary with a decay distance of d.

The surface C for the integral in eqn.6.28 has to avoid the singularity at $x_1 = x_2 = 0$ because the stress tensor diverges there. r_c is often called the core radius, but as we have argued the core has no radius in this theory. The meaning of r_c is more accurately described as the radius at which the elastic solution provides an acceptable description of the actual stresses near the dislocation. It is of order 1 nm in most crystalline materials. However, it is not necessarily the circular cross-section that has been assumed here and many other places. For example, in f.c.c. metals it is often found that the core is spread on the slip plane, so that it is much longer in that direction than it is normal to the slip plane by as much as a factor of ten or even more. The total energy per unit length of the dislocation is the sum of the elastic energy and the core energy per unit length.

The surface tension of a liquid arises because the surface of the liquid has an energy per unit area. If the surface is stretched more surface area is created by diffusion of atoms from beneath the surface which raises the energy of the system. The increase in energy may be thought of as the work done against the surface tension. Similarly a line tension may be associated with the energy per unit length of a dislocation: if there are no other forces acting on them dislocations will always seek to minimise their lengths.

The logarithmic singularity in the elastic energy per unit length of a dislocation is weak. Changing the outer radius R by an order of magnitude changes the elastic energy per unit length

by only a factor of $\ln 10$. Sometimes we need a rough estimate of the energy of a dislocation per unit length for back-of-an-envelope calculations, and then we use μb^2. This is also a useful approximation for the line tension of a dislocation. It is of order 0.1 to 1 eV/Å. This is also the order of magnitude of the energy per unit length of the core.

The energy of a dislocation loop is also given by eqn.6.28 where the surface C is that shown in Fig.6.6. The energy of the loop is then:

$$E_{el}^{loop} = \frac{1}{2}\int_{\Sigma^+} \sigma_{ij} b_i n_j \mathrm{d}S \tag{6.32}$$

where the integral is taken over the positive side of the cut surface inside the loop. This expression may be understood as the work done against the self-stress of the loop when it is created by increasing its Burgers vector from zero to the final b_i. By the conservation of energy this work becomes the elastic energy of the medium.

6.13 The Frank-Read source

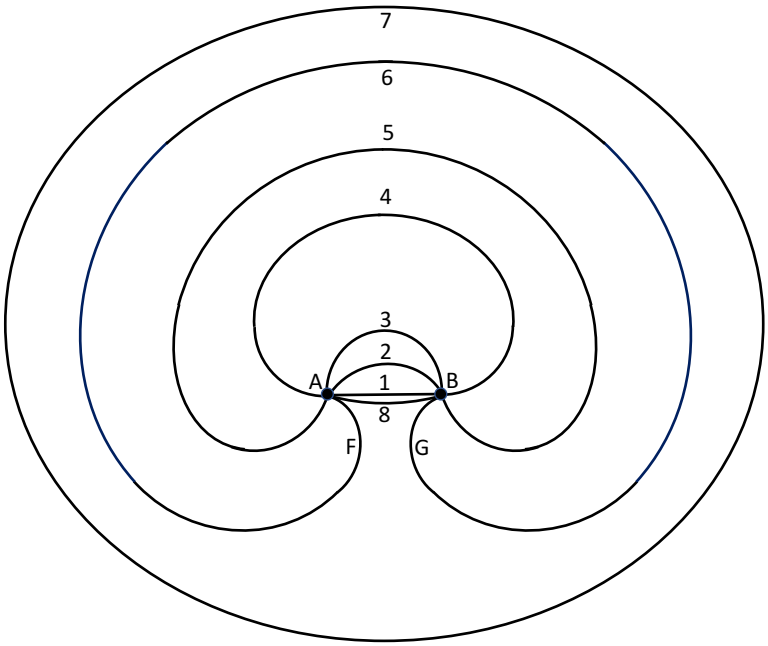

Figure 6.9: Schematic illustration of the operation of a Frank-Read source. A segment of dislocation line is pinned at A and B (configuration 1). Under the action of an applied shear stress on the slip plane in the direction of the Burgers vector the dislocation segment bows (configuration 2) against the line tension tending to keep it straight. Eventually a critical configuration is reached, configuration 3, where the radius of curvature of the dislocation segment is a minimum. The segment continues to expand (configurations 4, 5). Segments F and G have opposite line senses and attract each other. When they meet a loop, configuration 7, is liberated and expands under the action of the applied stress. A segment, configuration 8, is left behind and returns to AB and the process starts again.

For many years after it was recognised that dislocations are the agents of plastic deformation in metals it was not clear how they were created. But since the advent of electron microscopy in the

late 1950s there have been many observations of dislocations being produced inside crystals. One of the most commonly observed sources was proposed before it was observed by Frank and Read[22], and is known as a Frank-Read source[23].

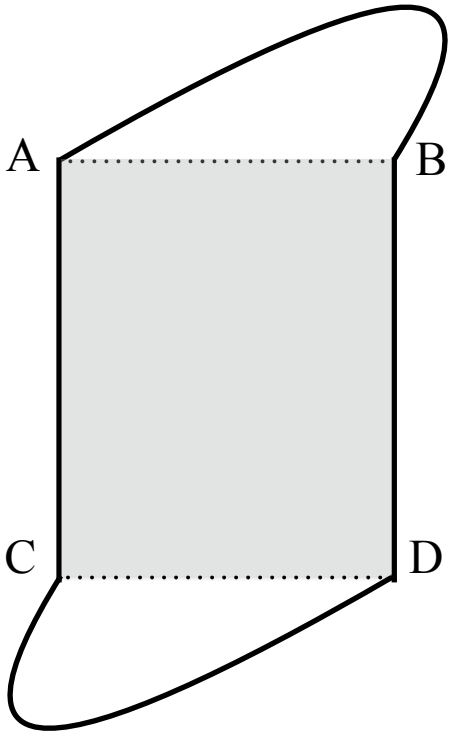

Figure 6.10: A rectangular prismatic loop ABCD with Burgers vector normal to the page initially occupies the shaded area. A shear stress is applied in the direction of the Burgers vector on planes containing the Burgers vector and the lines AB and CD. Segments AB and CD bow under the influence of this applied shear stress. However, segments AC and BD experience no resolved shear stress and remain static. Segments AB and CD may then operate as Frank-Read sources of loops, as illustrated in Fig.6.9.

Fig.6.9 illustrates the operation of a Frank-Read source. We consider a segment of a dislocation pinned at A and B. There are many ways the dislocation could be pinned at two points. In the paper by Frank and Read they considered a rectangular prismatic loop ABCD with Burgers vector normal to the plane of the loop, see Fig.6.10. A pure shear stress on the plane containing the Burgers vector and the line segment AB will make segments AB and CD move in opposite directions, but the

[22] F. C. Frank and W. T. Read, Phys. Rev. **79**, 722 (1950). Available online at `http://doi.org/10.1103/PhysRev.79.722`

[23] There is an entertaining account by Sir Charles Frank of how he and Thornton Read developed the idea of their dislocation source independently and precisely simultaneously in Proc. R. Soc. Lond. A **371**, 136 (1980), available online at: `http://dx.doi.org/10.1098/rspa.1980.0069`.

segments AD and BC will experience no Peach-Koehler force and remain static. The result is that the segments AB and CD are pinned at their ends.

Let τ be the resolved shear stress on the slip plane in the direction of the Burgers vector of the segment AB. The Peach-Koehler force acting on the segment is then τb where, as usual, b is the magnitude of the Burgers vector. This force acts in a direction normal to the line and the dislocation bows out between the pinning points (see configuration 2 in Fig.6.9). As a result the dislocation line length increases and this is opposed by the line tension, T. As the radius of curvature of the bowed segment decreases the stress required to make it bow further increases. Eventually a critical configuration is reached (configuration 3) where the radius of curvature is a minimum and the bowed segment expands with no further increase in the applied stress required. The segments F and G (see Fig.6.9) have opposite line senses and they attract each other and annihilate. This reaction liberates a loop (configuration 7) which then expands freely under the influence of the applied stress leaving behind a segment (configuration 8) which returns to the configuration AB at the beginning of the operation of the source. The process then repeats sending out a succession of loops into the slip plane. Eventually these loops meet obstacles such as grain boundaries where they may form a 'pile-up'. The dislocations in the pile-up exert a stress on the source, which is called a 'back stress', which may eventually prevent it from operating without increasing the applied stress further.

It is instructive to derive an approximate expression for the stress required to operate a Frank-Read source. This is a good example of a 'back-of-an-envelope' estimate that provides insight. Let the length of the pinned segment AB be L. We assume that when the dislocation starts to bow it forms the arc of a circle with a radius R. An element dl of the arc experiences an outward force due to the applied stress equal to $\tau b\mathrm{d}l$. It also experiences an inward force due to the line tension, given by $T\mathrm{d}l/R$ where $T \approx \mu b^2$. At equilibrium $\tau \approx \mu b/R$. As the segment bows further R decreases and τ increases until the critical configuration is reached where R is a minimum. This happens when the bowed segment is a semi-circle, with $R = L/2$. Thus, the minimum stress required to operate the source is $\tau_{min} \approx 2\mu b/L$ or $\mu b/L$ since this is only an order of magnitude estimate.

Efforts have been made to improve on this rough estimate. They include replacing the line tension approximation with an evaluation of the dislocation self-interactions when it bows, using anisotropic elasticity and including a friction stress that must overcome before a dislocation will move. These are all possible but much more difficult than our simple estimate.

The relationship $\tau \approx \mu b/L$ provides understanding in other contexts, and it is arguably one of the most useful in the theory of dislocations. Here are three examples:

- *Precipitation hardening*. One way metals are made stronger is by alloying them with elements that result in a dispersion of second phase particles. Dislocations moving in their slip planes encounter these particles. If the particles are sufficiently large that dislocations cannot cut through them they bow out between them and proceed on the slip plane after leaving a loop around each precipitate. The critical stress required for this process is of order $\mu b/L$ where L is the average separation of the precipitates. This is a key relationship in designing age-hardened alloys.

- *Work hardening*. Another way metals are made stronger is by deforming them plastically. This is called work hardening. It arises because dislocations moving on one slip plane encounter dislocations moving on inclined slip planes, as a result of which a variety of obstacles may form that impeded slip on both slip planes. Further slip then proceeds by dislocations bowing out between these obstacles. If L is the separation between the obstacles then the stress required for further slip is again of order $\mu b/L$. The spacing L is related to the dislocation density ρ, which is defined as the number of dislocations crossing unit area or equivalently the total dislocation length per unit volume: $\rho \approx 1/L^2$. Therefore the

stress required for dislocations to glide varies as $\mu b/L \approx \mu b\sqrt{\rho}$. This relationship was first proposed by G I Taylor in his paper of 1934 where he proposed dislocations as the agents of plasticity.

- *Plasticity in nanocrystals*. We saw at the beginning of this chapter that dislocations are the agents of plasticity because the stress required to slide an entire plane of atoms within a crystal over an adjacent plane is far too large. But if the area of the plane where slip occurs is very small, there might be a transition from slip mediated by dislocations to 'block slip' where an entire plane of atoms *can* slide over another. If a dislocation is introduced into cubic crystal of side L it will tend to be pinned by the surfaces. The stress required to make it bow out will be of order $\mu b/L$. Thus if $L \approx 10-100b$ the stress required to move the dislocation becomes comparable to that required for block slip.

6.14 Problem set 6

1. *Interaction energy of small prismatic loops*. Consider the interaction energy between two planar, small, prismatic loops A and B. In these loops the Burgers vector is parallel or anti-parallel to the loop normal. Loop A is at the origin of a Cartesian coordinate system and loop B is at $\mathbf{x}$, where $\mathbf{x} = x\hat{\mathbf{x}}$ is large compared to the sizes of the loops. Let the areas, Burgers vectors and unit normals of the loops be $A^{(A)}, \mathbf{b}^{(A)}, \hat{\mathbf{n}}^{(A)}$ and $A^{(B)}, \mathbf{b}^{(B)}, \hat{\mathbf{n}}^{(B)}$. The second derivative of the isotropic elastic Green's function is as follows:

$$\begin{aligned} G_{ik,jl}(\mathbf{x}) &= \frac{1}{16\pi\mu(1-\nu)x^3} \times \\ &\{(3-4\nu)\delta_{ik}\left(3\hat{x}_l\hat{x}_j - \delta_{lj}\right) \\ + \quad & 15\hat{x}_i\hat{x}_j\hat{x}_k\hat{x}_l - 3(\delta_{ij}\hat{x}_k\hat{x}_l + \delta_{il}\hat{x}_j\hat{x}_k + \delta_{jl}\hat{x}_i\hat{x}_k \\ + \quad & \delta_{kj}\hat{x}_i\hat{x}_l + \delta_{kl}\hat{x}_i\hat{x}_j) + (\delta_{il}\delta_{kj} + \delta_{kl}\delta_{ij})\}. \end{aligned} \tag{6.33}$$

Show that the interaction energy between the loops is as follows:

$$\begin{aligned} E_{int}^{(AB)} &= \frac{\mu b^{(A)} b^{(B)} A^{(A)} A^{(B)}}{4\pi(1-\nu)r^3}\{15(\hat{n}^{(A)}.\hat{r})^2(\hat{n}^{(B)}.\hat{r})^2 \\ - \quad & (4\nu-1) - 12\nu(\hat{n}^{(A)}.\hat{n}^{(B)})(\hat{n}^{(A)}.\hat{r})(\hat{n}^{(B)}.\hat{r}) \\ - \quad & (1-2\nu)[3(\hat{n}^{(B)}.\hat{r})^2 + 3(\hat{n}^{(A)}.\hat{r})^2 + 2(\hat{n}^{(A)}.\hat{n}^{(B)})^2]\}. \end{aligned} \tag{6.34}$$

2. In eqn.4.13 the displacement field of an infinite planar fault was derived:

$$u_i(\mathbf{x}) = -\int_{fault} G_{ij,l'}(\mathbf{x}-\mathbf{x}')\, c_{jlmp}\, t_m\, n_p\, \mathrm{d}^2x', \tag{6.35}$$

where $\mathbf{t}$ is the translation of the medium on the negative side of the fault relative to that on the positive side. In isotropic elasticity we have:

$$c_{jlmp}G_{ij,l'}(\mathbf{X}) = \frac{1}{8\pi(1-\nu)}\left[(1-2\nu)\frac{\delta_{mi}X_p + \delta_{pi}X_m - \delta_{mp}X_i}{X^3} + 3\frac{X_mX_pX_i}{X^5}\right], \tag{6.36}$$

where $\mathbf{X} = \mathbf{x} - \mathbf{x}'$.

If the fault is in the plane $x_3 = 0$ verify that eqn.6.35 yields $u_i(\mathbf{x}) = -\frac{1}{2}\mathrm{sgn}(x_3)t_i$.

3. Using Volterra's formula for the displacement field of a dislocation in the form:

$$u_i(\mathbf{x}) = -c_{jlmp}\, b_m \int_{\mathscr{S}^+} G_{ij,l'}(\mathbf{x}-\mathbf{x}')\, n'_p \,\mathrm{d}S',$$

and using eqn.6.36 show that, with the cut in the half-plane $x_2 = 0, x_1 \geq 0$, the displacement field of a screw dislocation in isotropic elasticity is as follows:

$$\begin{aligned} u_1(x_1,x_2) &= 0 \\ u_2(x_1,x_2) &= 0 \\ u_3(x_1,x_2) &= \frac{b}{2\pi}\tan^{-1}\left(\frac{x_2}{x_1}\right). \end{aligned}$$

4. Using Mura's formula, eqn.6.25, in isotropic elasticity show that the strain and stress fields of a screw dislocation lying along the x_3-axis with Burgers vector $\mathbf{b} = [0,0,b]$ are as follows:

$$\begin{aligned} e_{11} &= e_{22} = e_{33} = e_{12} = 0 \\ e_{13} &= -\frac{b}{4\pi}\frac{x_2}{x_1^2+x_2^2} \\ e_{23} &= \frac{b}{4\pi}\frac{x_1}{x_1^2+x_2^2} \\ \sigma_{11} &= \sigma_{22} = \sigma_{33} = \sigma_{12} = 0 \\ \sigma_{13} &= -\frac{\mu b}{2\pi}\frac{x_2}{x_1^2+x_2^2} \\ \sigma_{23} &= \frac{\mu b}{2\pi}\frac{x_1}{x_1^2+x_2^2} \end{aligned}$$

Verify that your answer is consistent with the displacement field of the screw dislocation derived in the previous question.

5. Calculate the elastic energy of a screw dislocation in isotropic elasticity two ways:
(i) by integrating the elastic energy density $\frac{1}{2}\sigma_{ij}e_{ij}$ using the stress and strain tensors derived in the previous question.
(ii) by using eqn.6.29.

6. A crystal contains screw dislocations with Burgers vectors $\pm\mathbf{b}$ gliding on a set of primary slip planes. Let the dislocations lie along the x_3-axis and let the normal to the primary slip planes be $[010]$. A screw dislocation with Burgers vector $\mathbf{b} = [0,0,b]$ is pinned at the origin of the coordinate system. A second screw dislocation with Burgers vector $\mathbf{b} = [0,0,-b]$ is gliding on a parallel slip plane. The distance between the slip planes of the two dislocations is D. Assuming the mobile screw dislocation remains on the same slip plane show that the

minimum applied shear stress required to enable it to continue gliding past the static screw dislocation is $\sigma_{23}^* = \mu b/(4\pi D)$.

Suppose the mobile screw dislocation is able to cross-slip onto a secondary slip plane making an angle α with the primary slip plane. Show that mobile screw dislocation will cross-slip and annihilate the static dislocation at the origin at a value of σ_{23} smaller than σ_{23}^*.

7. A crystal contains edge dislocations with Burgers vectors $\pm\mathbf{b}$ gliding on a set of primary slip planes. Let the dislocations lie along the x_3-axis and let the normal to the primary slip planes be $[010]$. An edge dislocation with Burgers vector $\mathbf{b} = [b,0,0]$ is pinned at the origin of the coordinate system. A second edge dislocation with Burgers vector $\mathbf{b} = [b,0,0]$ is gliding on a parallel slip plane. The distance between the slip planes of the two dislocations is D. Show that the position of stable equilibrium of the second dislocation is at $x_1 = 0, x_2 = D$. If now the Burgers vector of the second dislocation is $\mathbf{b} = -[b,0,0]$ show that it has two positions of stable equilibrium at $x_1 = \pm D, x_2 = D$.

8. Stress field of a symmetric tilt boundary.

This question illustrates how dislocations may organise themselves into configurations where they screen their elastic fields, reducing the overall elastic energy.

A small angle symmetric tilt grain boundary in the plane $x_1 = 0$ comprises an infinite array of edge dislocations with Burgers vector $[b,0,0]$. The dislocation lines are parallel to the x_3-axis and their positions along the x_2-axis are $x_2 = 0, \pm p, \pm 2p, \pm 3p, \ldots, \pm\infty$. Using the components of the stress tensor for an edge dislocation given in eqn.6.27 show that the non-zero stress components of the grain boundary are:

$$\begin{aligned}
\sigma_{11}(x_1,x_2) &= -\frac{\mu b p}{2\pi(1-\nu)} \sum_{n=-\infty}^{\infty} (X_2 - n) \left(\frac{3X_1^2 + (X_2-n)^2}{\left(X_1^2 + (X_2-n)^2\right)^2} \right) \\
\sigma_{12}(x_1,x_2) &= \frac{\mu b p}{2\pi(1-\nu)} \sum_{n=-\infty}^{\infty} X_1 \left(\frac{X_1^2 - (X_2-n)^2}{\left(X_1^2 + (X_2-n)^2\right)^2} \right) \\
\sigma_{22}(x_1,x_2) &= \frac{\mu b p}{2\pi(1-\nu)} \sum_{n=-\infty}^{\infty} (X_2 - n) \left(\frac{X_1^2 - (X_2-n)^2}{\left(X_1^2 + (X_2-n)^2\right)^2} \right) \\
\sigma_{33}(x_1,x_2) &= -\frac{\mu b p \nu}{\pi(1-\nu)} \sum_{n=-\infty}^{\infty} \frac{X_2 - n}{X_1^2 + (X_2-n)^2}
\end{aligned}$$

where $X_1 = x_1/p$ and $X_2 = x_2/p$.

The sums may be evaluated as contour integrals using the Sommerfeld-Watson transformation. For example,

$$\sum_{n=-\infty}^{\infty} \frac{1}{n+a} = \frac{1}{2\pi i} \oint_C \pi \cot(\pi z) \frac{1}{z+a} \mathrm{d}z = \pi \cot \pi a,$$

where the contour includes all the poles of $\cot(\pi z)$ along the real axis where $z = n$, but excludes the pole at $z = a$ and is closed by a circle at infinity. The result holds for real or

complex a. We may use this result to derive all the sums we need to evaluate the stress components for the grain boundary. For example, since

$$\frac{1}{n+X_2+iX_1}+\frac{1}{n+X_2-iX_1}=\frac{2(n+X_2)}{(n+X_2)^2+X_1^2}$$

we deduce that

$$\sum_{n=-\infty}^{\infty}\frac{n+X_2}{(n+X_2)^2+X_1^2}=\frac{\pi\sin(2\pi X_2)}{\cosh(2\pi X_1)-\cos(2\pi X_2)}.$$

Hence show that the non-zero components of the stress tensor associated with the grain boundary are as follows:

$$\begin{aligned}
\sigma_{11} &= -\frac{\mu b}{2(1-\nu)p}\frac{\sin(2\pi X_2)\left[\cosh(2\pi X_1)-\cos(2\pi X_2)+2\pi X_1\sinh(2\pi X_1)\right]}{\left(\cosh(2\pi X_1)-\cos(2\pi X_2)\right)^2}\\
\sigma_{12} &= \frac{\pi\mu b}{(1-\nu)p}\frac{X_1\left[\cosh(2\pi X_1)\cos(2\pi X_2)-1\right]}{\left(\cosh(2\pi X_1)-\cos(2\pi X_2)\right)^2}\\
\sigma_{22} &= -\frac{\mu b}{2(1-\nu)p}\frac{\sin(2\pi X_2)\left[\cosh(2\pi X_1)-\cos(2\pi X_2)-2\pi X_1\sinh(2\pi X_1)\right]}{\left(\cosh(2\pi X_1)-\cos(2\pi X_2)\right)^2}\\
\sigma_{33} &= -\frac{\mu b\nu}{(1-\nu)p}\frac{\sin(2\pi X_2)}{\left(\cosh(2\pi X_1)-\cos(2\pi X_2)\right)}
\end{aligned}$$

When $|x_1|>p$ show that these stress components are approximately proportional to $e^{-2\pi|x_1|/p}$.

Show that in the limit $p\to\infty$ these stress components become those of an isolated dislocation, given in eqn.6.27.

9. Having derived the stress component $\sigma_{12}(x_1,x_2)$ for the symmetrical tilt grain boundary in the previous question we may use it to calculate the energy of the boundary. Let the cut associated with each edge dislocation at $x_1=0,x_2=np$ be in the half-plane $x_2=np,x_1\geq 0$. Following the same argument using the divergence theorem to derive eqn.6.29, where the contour C now involves an infinite number of circuits around the cuts and the dislocations in the grain boundary, show that the elastic energy of the grain boundary is as follows:

$$E_{GB}=\frac{1}{p}\left[\frac{1}{2}\int_{r_c}^{R}\sigma_{12}(x_1,0)\,b\,\mathrm{d}x_1+E_c\right]$$

where E_c is the energy per unit length of the material inside the radius r_c of each dislocation that cannot be described with elasticity. It is assumed that E_c does not vary with the misorientation angle θ. This assumption is reasonable provided θ is small. In that case $\theta=b/p$ is also a good approximation.

Given the standard integral

$$\int\frac{u}{\sinh^2 u}\mathrm{d}u=\ln(\sinh u)-u\coth u$$

show that

$$E_{GB} = \theta\left[\left\{\frac{E_c}{b} + \frac{\mu b}{4\pi(1-\nu)}\ln\left(\frac{eb}{2\pi r_c}\right)\right\} - \frac{\mu b}{4\pi(1-\nu)}\ln\theta\right]$$

This equation has the form $E_{GB} = \theta(A - B\ln\theta)$ where A and B are constants:

$$A = \frac{E_c}{b} + \frac{\mu b}{4\pi(1-\nu)}\ln\left(\frac{eb}{2\pi r_c}\right)$$

$$B = \frac{\mu b}{4\pi(1-\nu)}$$

It is known as the Read-Shockley[24] formula[25].

10. In this question we repeat the calculation of the energy of a small angle symmetrical tilt grain boundary but in a more heuristic but insightful way. The insight is to exploit the mutual screening of the elastic fields of the edge dislocations it contains. The larger radius R in eqn.6.30 for the energy of an isolated edge dislocation may be taken as half the spacing p of the dislocations in the boundary. Show that the energy per unit area of the grain boundary is then

$$E_{GB} \approx \frac{1}{p}\left[\frac{\mu b^2}{4\pi(1-\nu)}\ln\left(\frac{p}{2r_c}\right) + E_c\right]$$

where E_c is the energy of the material inside the radius r_c which cannot be described with elasticity. As before, the angle θ of misorientation across the boundary is approximately b/p. Show that E_{GB} has the form

$$E_{GB} \approx \theta(A - B\ln\theta) \tag{6.37}$$

where A and B are constants with the dimensions of energy per unit area:

$$A = \frac{E_c}{b} + \frac{\mu b}{4\pi(1-\nu)}\ln\left(\frac{b}{2r_c}\right)$$

$$B = \frac{\mu b}{4\pi(1-\nu)}$$

This heuristic solution is very close to the more rigorous solution in the previous question.

[24] William Bradford Shockley (1910-1989) U.S. Nobel prize winning physicist
[25] W. T. Read and W. Shockley, Phys. Rev. **78**, 275 (1950)

7. Atomistic-continuum models of dislocations

8. Continuous distributions of dislocations

9. The energy-momentum tensor

9.1 Interaction energy

10. Open questions

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