

Name: Antriksh Dhand

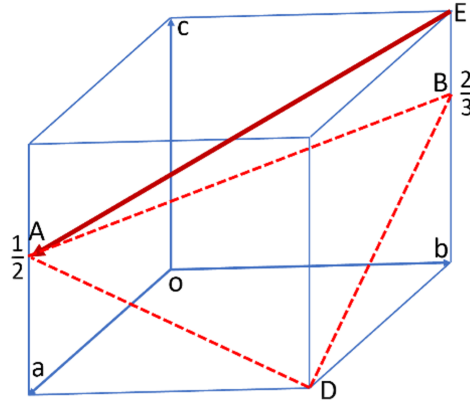
Student ID: 510415022

Tutor's Name: Naveed Khan

Tutorial Class: TUT05, Tuesday 2-4pm

Question 1

Determine the index for the direction EA and the Miller index for the plane ABD shown below.
[20%]



Q1.1 Direction of EA

Consider a right-handed xyz coordinate system with origin at point $O(0, 0, 0)$. Then, $E = (0, 1, 1)$ and $A = (1, 0, \frac{1}{2})$. So tail coordinates are

$$x_1 = 0a \quad y_1 = 1b \quad z_1 = 1c \quad (1)$$

And head coordinates are

$$x_2 = 1a \quad y_2 = 0b \quad z_2 = \frac{1}{2}c \quad (2)$$

For the direction EA , subtracting tail coordinates from head coordinates, we have

$$u = x_2 - x_1 = 1a - 0a = 1a \quad (3)$$

$$v = y_2 - y_1 = 0b - 1b = -1b \quad (4)$$

$$w = z_2 - z_1 = \frac{1}{2}c - 1c = -\frac{1}{2}c \quad (5)$$

Normalising these in terms of unit cell dimensions results in

$$u = 1 \quad v = -1 \quad w = -\frac{1}{2} \quad (6)$$

Now multiplying each by a factor of 2 to result in smallest integer values:

$$u = 2 \quad v = -2 \quad w = -1 \quad (7)$$

Therefore the EA direction index can be written as $[2\bar{2}\bar{1}]$.

Q1.2 Miller index of plane ABD

Take the origin to be at point $b(0,1,0)$. Then, with respect to this new origin, $A = (1, -1, \frac{1}{2})$, $D = (1, 0, 0)$ and $B = (0, 0, \frac{2}{3})$. From the diagram, it is clear that the intersection of the plane with the x - and z - axes are points D and B respectively.

Let the intersection of the plane with the y -axis be the point $F = (0, \lambda, 0)$, $\lambda \in \mathbb{R}$. Note that the plane $ABFD$ forms a parallelogram, and therefore $AD \parallel BF$. That is, the gradient of line BF is identical to the gradient of line AD :

$$m_{BF} = m_{AD} = -\frac{1}{2} \quad (8)$$

So the equation of the line BF is

$$z = -\frac{1}{2}y + \frac{2}{3} \quad (9)$$

To find y -intercept, put $z = 0$:

$$\frac{1}{2}y = \frac{2}{3} \quad (10)$$

$$\implies y = \lambda = \frac{4}{3} \quad (11)$$

Hence, point $F = (0, \frac{4}{3}, 0)$ and the intercepts of the plane with the axes are:

$$x = 1 \quad y = \frac{4}{3} \quad z = \frac{2}{3} \quad (12)$$

Taking reciprocals,

$$h = 1 \quad k = \frac{3}{4} \quad l = \frac{3}{2} \quad (13)$$

Reducing to smallest integer value by multiplying by 4,

$$h = 4 \quad k = 3 \quad l = 6 \quad (14)$$

So the Miller indices for the plane are $(4\ 3\ 6)$.

Question 2

Please list the indices of all planes that belong to the $\{120\}$ family in a tetragonal crystal with lattice parameters $a = b \neq c$ and $\alpha = \beta = \gamma = 90^\circ$. [10%]

Note that for the (120) plane in the $\{120\}$ family, $h = 1$, $k = \frac{1}{2}$ and $l = \infty$. That is, the point of intersection of the plane with the x - and y - axes is at 1 and $\frac{1}{2}$ respectively, and the plane does not intersect with the z -axis. The (120) plane is illustrated in Figure 1.

Now, a family of planes are a group of planes which all share the same atomic packing (i.e. they are *crystallographically equivalent*). As seen in Figure 1, the plane only intersects with 2 atoms at B and C . Any plane that can be formed through a translation or rotation of this plane, with the exact same dimensions and exact same atomic packing (i.e. passing through two atoms), will be a part of the $\{120\}$ family.¹ In total there are 4 such planes and these are illustrated in Figures 1 and 2. These are

$$\{120\} = (120), (\bar{1}20), (2\bar{1}0), (210) \quad (15)$$

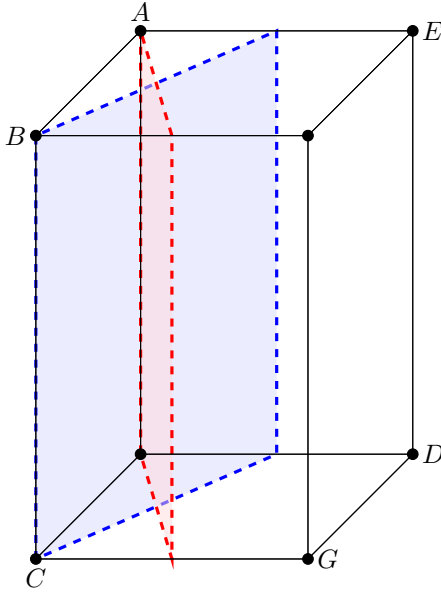


Figure 1: The (120) and $(\bar{1}20)$ planes in blue and red respectively.

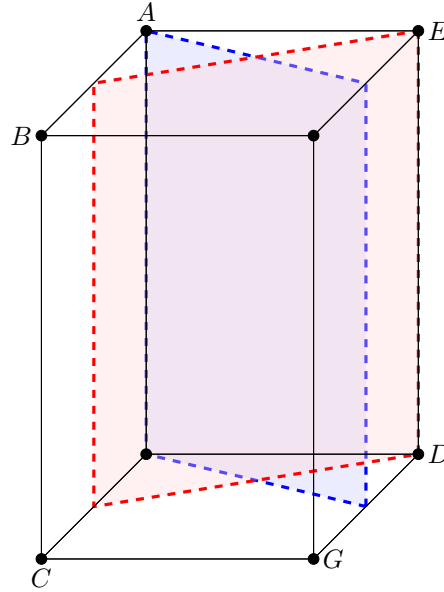


Figure 2: The $(2\bar{1}0)$ and (210) planes in blue and red respectively.

¹Note that this also includes parallel planes, however as these have the same Miller indices as the original, we do not differentiate them.

Question 3

Please provide the definition of the following terms: isotropy, anisotropy, polymorphism, and allotropy. [10%]

Anisotropy: Anisotropy is a property where certain materials exhibit variations in physical properties along different molecular axes i.e. the *directionality* of properties. Anisotropy is associated with the variance of atomic or ionic spacing with crystallographic direction. For example, the measured modulus of elasticity or electrical conductivity of a material may differ based on which crystallographic direction it is measured from (e.g. $[100]$ vs $[111]$).

Isotropy: Isotropy is the opposite of anisotropy — it is the phenomenon where measured properties of a material are independent of the direction of measurement.

Polymorphism: Polymorphism is when one material has two or more distinct crystal structures. It is a general term which can be used for materials composed of one or multiple elements. For example, Fe_2O_3 (iron oxide) has three phases: a rhombohedral α phase which is present in ambient conditions, a body-centered cubic β phase present at higher temperatures but below 773K, and a cubic-structured γ phase present at up to 933K.

Allotropy: Allotropy is a subset of polymorphism that only applies to pure elements. There are plenty of examples of this, perhaps the most well known being carbon which can assume many different structures such as those found in graphite, diamond, and carbon nanotubes. Another example is pure iron which assumes a body-centered cubic structure at up to 912°C, a face-centered cubic structure at temperatures between 912°C and 1394°C, and once again returns to a body-centered cubic structure at temperatures higher than 1394°C but lower than melting point.

Question 4

Please list all the crystalline defects that you learned in Chapter 4. [10%]

A crystalline defect is any place in the crystal structure where the periodic array of atoms stop. These defects are often categorised by their dimension.

Q4.1 Zero-dimensional defects

These are also known as “point defects.” These include:

- **Vacancy atoms/vacancies:** a vacant atomic site in a structure which is usually filled. These cause the distortion of planes in the lattice, increasing the total system’s energy.
- **Self-interstitials:** atoms in the crystal that are crowded into an interstitial site (a small void space which under ordinary circumstances is unoccupied). These introduce much more distortion into the atom and thus are quite uncommon compared to vacancies.
- Formation of a **solid solution** when solute atoms are added to a host material.
 - *Substitutional atoms:* where solute atoms replace host atoms. This requires both host and solute atoms to have similar atomic radii, electro-negativities, valencies and have identical crystal structures.
 - *Interstitial atoms:* where solute atoms fill the voids or *interstices* among the host atoms. This requires the size of the solute atoms to be much smaller than the host atoms.

- Formation of a **second phase**: when you mix two elements together and observe periodicity at some location inside the crystal structure. Also known as a *precipitate*.

Q4.2 One-dimensional defects

These are also known as “linear defects” or “dislocations.” Dislocations are defects around which some of the atoms are misaligned. There are two main types of dislocations, however usually these occur together in what is known as a **mixed dislocation**.

- **Edge dislocation**: where an extra half-plane of atoms are inserted in a crystal structure, with localised distortion around the dislocation line.
- **Screw dislocation**: analogous to a shear stress shifting/translating one region of the crystal away from the other.

Q4.3 Two-dimensional defects

Often referred to as “planar” or “interfacial” defects, these are two-dimensional boundaries which separate regions of the material with different crystal structures.

- **External surface**: the outer wall of the crystal marks the termination of the periodic array of atoms and therefore is a type of defect.
- **Grain boundary**: these occur when there is an atomic mismatch between the crystalline orientation of one grain to that of an adjacent one.
- **Twin boundary**: a twin boundary is a special type of grain boundary where atoms on one side are essentially a reflection of the atom positions on the other side. This is known as “twinning.”
- **Stacking faults**: All cubic structures are made up of the stacking of close-packed planes. A stacking fault arises when there is a discontinuity in the periodicity of the stacking e.g. for an *ABCABCABC* structure, a stacking fault arises if one or more of those layers is missing or there is an extra one such as *ABABCABBC*.

Q4.4 Three-dimensional defects

Known as “bulk” or “volume” defects. These include pores, cracks, foreign inclusions and other phases.

Question 5

Iron (Fe) can have either a face-centered cubic (FCC) structure or a body-centered cubic (BCC) structure. The lattice parameter for FCC Fe and BCC Fe is 0.3571 nm and 0.2866 nm, respectively. Please calculate the radius of Fe in the two structures by assuming the hard sphere model in which the nearest atoms touch each other. Please also calculate the linear density along the close-packed directions in the FCC and BCC Fe. [20%]

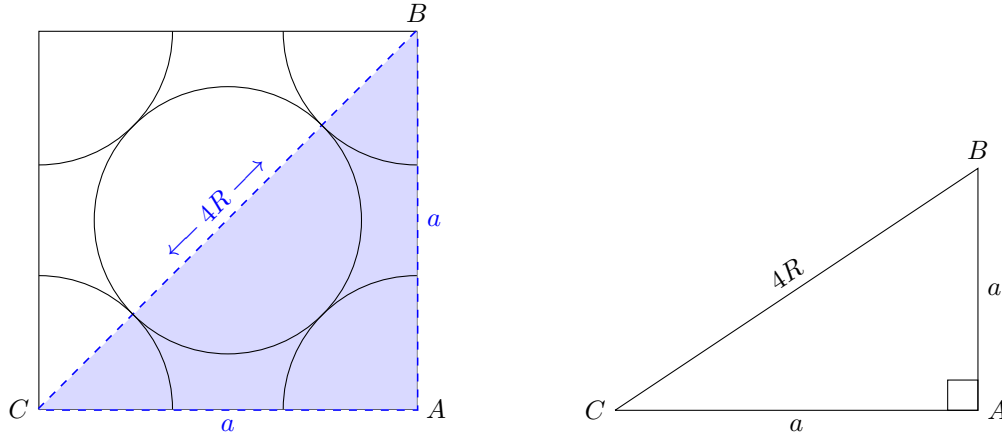
Q5.1 FCC Fe structure

Figure 3: Generic FCC face structure

In an FCC structure, assuming the hard sphere model, atoms touch each other along the cube face diagonal. Therefore, from applying Pythagoras' Theorem to Figure 3, we have that

$$a^2 + a^2 = (4R)^2 \quad (16)$$

$$2a^2 = 16R^2 \quad (17)$$

$$R^2 = \frac{1}{8} a^2 \quad (18)$$

$$\Rightarrow R = \frac{1}{2\sqrt{2}} a \quad (19)$$

The lattice parameter a for FCC iron is given as $a = 0.3571$ nm. Therefore

$$R[\text{Fe}]_{\text{FCC}} = \frac{1}{2\sqrt{2}} \cdot (0.3571 \times 10^{-9}) \quad (20)$$

$$= 1.2625... \times 10^{-10} \quad (21)$$

$$\approx 0.126 \times 10^{-9} \text{ m} \quad (22)$$

That is, the radius of the iron atom in face-centered cubic structure is approximately 0.126 nm.

Now, the close-packed directions of an atom are the directions in which atoms are touching each other in the structure. In the FCC case, this is the direction $[110]$. Along this direction, as seen in

Figure 3, there are a total of 4 radii i.e. 2 diameters which corresponds to a total of 2 atoms centered on this specific direction vector. Therefore,

$$LD_{110} = \frac{\text{number of atoms}}{\text{length of vector}} \quad (23)$$

$$= \frac{2}{4R} \quad (24)$$

We know R from equation 21, and so

$$LD_{110} = \frac{1}{2 \cdot (1.2625... \times 10^{-10})} \quad (25)$$

$$= 3.96027... \times 10^9 \quad (26)$$

$$\approx 3.96 \text{ nm}^{-1} \quad (27)$$

That is, the linear density of the $[110]$ direction (the close-packed direction) of FCC iron is approximately 3.96 nm^{-1} .

Q5.2 BCC Fe structure

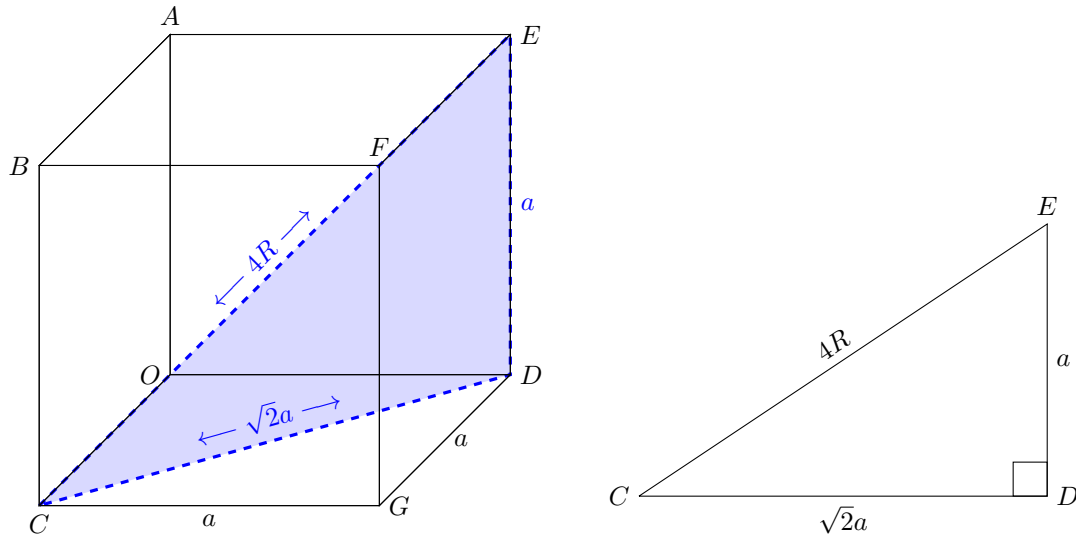


Figure 4: Generic BCC face structure

In an BCC structure, assuming the hard sphere model, atoms touch each other along the cube's diagonal. Looking at Figure 4 and applying Pythagoras' Theorem twice (first on the base to find the

hypotenuse $CD = \sqrt{2}a$ and then once again to find the cube's diagonal), we have:

$$(\sqrt{2}a)^2 + a^2 = (4R)^2 \quad (28)$$

$$3a^2 = 16R^2 \quad (29)$$

$$R^2 = \frac{3}{16} a^2 \quad (30)$$

$$\implies R = \frac{\sqrt{3}}{4} a \quad (31)$$

The lattice parameter a for BCC iron is given as $a = 0.2866 \text{ nm}$. Therefore

$$R [\text{Fe}]_{\text{BCC}} = \frac{\sqrt{3}}{4} \cdot (0.2866 \times 10^{-9}) \quad (32)$$

$$= 1.24101... \times 10^{-10} \quad (33)$$

$$\approx 0.124 \times 10^{-9} \text{ m} \quad (34)$$

That is, the radius of the iron atom in body-centered cubic structure is approximately 0.124 nm .

In the BCC case, the close-packed direction is $[111]$. Similar to the FCC case, there are 2 atoms centered on this direction vector. Therefore,

$$\text{LD}_{111} = \frac{2}{4R} \quad (35)$$

We know R from equation 34, and so

$$\text{LD}_{111} = \frac{1}{2 \cdot (1.24101... \times 10^{-10})} \quad (36)$$

$$= 4.02896... \times 10^9 \quad (37)$$

$$\approx 4.03 \text{ nm}^{-1} \quad (38)$$

That is, the linear density of the $[111]$ direction (the close-packed direction) of BCC iron is approximately 4.03 nm^{-1} .

Question 6

Please list four strategies for strengthening metallic materials. Briefly describe how these strategies can strengthen materials and provide empirical strengthening relationships. Please also briefly explain why metals with FCC structures are in general more ductile and present better formability than metals with HCP structures. [20%]

In order to strengthen a material, you must increase its resistance to plastic deformation. Plastic deformation itself occurs through dislocation motion. To illustrate this further, consider a generic edge dislocation. When an external shear stress is applied, the edge dislocation (along with all neighbouring planes) moves in the direction of the stress. If the applied stress is of great enough magnitude, the interatomic bonds of the plane adjacent to the extra half-plane are severed. The upper half of this adjacent plane then becomes the extra half-plane, with the bottom half linking up with the original dislocation. This process is repeated such that the extra half-plane, by the repeated and successive breaking and reforming of bonds, moves towards the surface of the crystal, ultimately emerging and forming an edge that is one atomic distance wide. It is this edge which, in a process termed as *slip*, forms a permanent (plastic) deformation.

It follows that in order to strengthen a material you must reduce the mobility of its dislocations.

Q6.1 Grain size reduction

A polycrystalline material is composed of a collection of multiple grains. The area which separates each grain from another, known as the *grain boundary*, contains some degree of atomic mismatch or *crystallographic misalignment*. This results in adjacent grains having different crystallographic orientations (see Figure 5).

Now, as described earlier, a dislocation must traverse the interior of the lattice and emerge onto the surface for plastic deformation to occur i.e. in a polycrystalline material, the slip motion (at some point) must take place across a grain boundary. However, the crystallographic misalignment within the grain boundary results in a discontinuity of slip planes from one grain to another. The slip plane is forced to change direction while traversing the grain boundary, a feat which becomes increasingly difficult as the misorientation of grains increases. In other words, the presence of a grain boundary impedes the dislocation motion.

The degree of misalignment across a grain boundary is usually quantified as the angle between them, termed a “high-angle grain boundary” or “small-angle grain boundary” (see Figure 5). Hence, in order to strengthen a metal, we want a) as many grains as possible and b) grains with a high-angle boundary. Luckily, both these conditions can be satisfied by simply reducing the size of each grain. In doing so, not only do you result in a larger number of planes in more crystallographic orientations, but on average, the angle across the grain boundary also increases.

This can also be seen in the empirical Hall-Petch equation:

$$\sigma_y = \sigma_0 + k_y d^{-1/2} \quad (39)$$

where d is the average grain diameter and σ_0 and k_y are constants for a particular material. So, as d decreases, σ_y increases, showing that by reducing the grain sizes in a polycrystalline material, the strength increases.

The reduction of grain sizes in a material is possible by regulating the rate of solidification from when the material is still in its liquid phase, or by plastically deforming the material and following it up with an appropriate heat treatment.

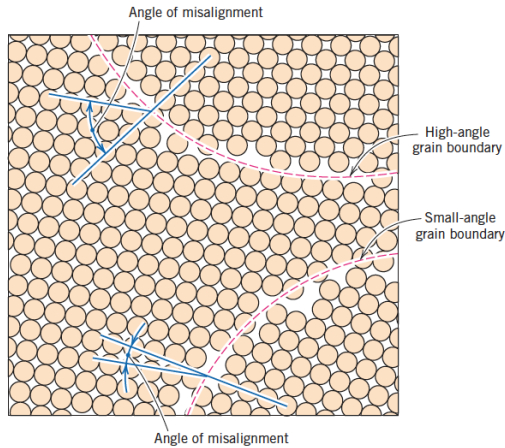


Figure 5: Adjacent grains in a polycrystalline material.

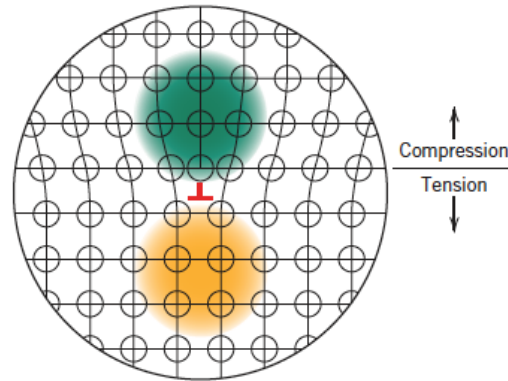


Figure 6: Typical lattice strains for an edge dislocation.

Q6.2 Solid-solution strengthening

The addition of impurity atoms into a metal can result in the formation of a *solid solution*, a structure where impurity atoms are randomly and uniformly dispersed within the lattice structure. Both substitutional and interstitial solid solutions actually hinder dislocation motion and thus are purposely introduced in metals in order to strengthen them.

Once again, consider a generic edge dislocation, specifically the existence of atomic lattice distortion around its dislocation line. This is to be expected — similar to how a block of butter seems to ‘cling’ to a knife cutting through it, the atoms around the extra half-plane above the slip line are in compression. Below the slip line, the atoms are in tension (see Figure 6). It is also possible to justify this through the model of equilibrium: atoms display a tendency to maintain their usual inter-atomic distance d_0 (also known as the *equilibrium inter-atomic distance*). When they are pushed apart to inter-atomic distance d due to the extra half-plane, a compressive strain acts to restore them to a distance d_0 :

$$\varepsilon_d = \frac{d - d_0}{d} \quad (40)$$

A converse argument can be made for atoms in tension below the slip plane. These compressive and tensile strains are known as *lattice strains* and can be modelled as a *strain field*.

These strain fields associated with dislocations become incredibly important when we see that impurity atoms in a solid solution *also* impose lattice strains on surrounding host atoms. It is when strain field interactions occur between dislocations and impurity atoms that dislocation motion is restricted, thus strengthening the metal.

For example, consider the interaction between the tensile strain field of a solute atom and the tensile strain field of a dislocation. This repulsion will actually impede the motion of a dislocation traversing through the crystal lattice. If the interaction was tensile/compressive, there will be an attraction, and a tendency for the dislocation line to remain close to the solute atom and not proceed further. In either case, the motion of the dislocation is impeded and the metal is strengthened.

Furthermore, solute atoms tend to diffuse to dislocations in such a way as to reduce the overall strain energy. Consider the lattice shown in Figure 6. Above the slip plane there is compression i.e. there is ‘too little space’ to fit the required atoms. Therefore, if the substitutional atom is smaller than

the host atom, it will tend to diffuse to a position above the slip plane, reducing the tensile strain as per equation 41. Similarly, larger impurity atoms will tend to diffuse to below the slip plane.

Finally, in a process known as *interstitial pinning* or *solute segregation* (related to the concept of the Cottrell atmosphere), interstitial impurity atoms are able to act as an ‘anchor’, hindering dislocation motion. For example, in many carbon steels where carbon atoms form an interstitial solid solution, in order to lower the overall lattice strain energy the carbon atoms diffuse towards dislocations. They thereby become ‘pinned’ and required a large force to move them. This large force is what we observe as the upper yield point in a stress-strain graph of such a material. Indeed, it requires much greater energy to move a dislocation in a lattice experiencing this phenomenon, hence strengthening the metal.

Empirically, the relationship between metal strengthening and impurity atoms has been stated as

$$\sigma_y \propto \sqrt{C} \quad (41)$$

where σ_y is the yield strength of a metal and C is the concentration of an impurity in that metal.

Q6.3 Strain hardening

Also known as work hardening or cold working.

Strain hardening is the phenomenon where a ductile metal becomes harder and stronger as it is plastically deformed at room temperature. To understand this phenomenon, it is necessary to give a brief overview of dislocation multiplication.

It has been observed experimentally that the dislocation density, given by Equation 43, is much greater for a plastically deformed material than that of an undeformed solid.

$$\rho_{\perp} = \frac{\text{total dislocation length}}{\text{volume}} \quad (42)$$

But this seems contradictory to the fact that plastic deformation requires dislocations to traverse through the lattice structure and appear on the outside as a slip step. Shouldn’t dislocation density *decrease* after plastic deformation? Scientists Frank and Read herein proposed the existence of sources of dislocations inside crystals, which operate during plastic deformation and have the net effect of increasing the dislocation density. This is known as *dislocation multiplication*, where the Frank-Read sources are actually pre-existing dislocations.

So when plastic deformation occurs, the dislocation density increases because of dislocation multiplication, decreasing the average separation distance between dislocations. This brings dislocations closer to one another, allowing them to experience dislocation-dislocation strain field interactions. A large majority of these interactions are repulsive, hindering the motion of a dislocation as it is trying to traverse through the crystal lattice. If an interaction happens to be attractive, dislocation annihilation will occur, leading to the formation of a perfect crystalline lattice in place of the dislocations. Either way, the motion of a particular dislocation is impeded by the very presence of other dislocations. Hence, the yield strength of a metal increases as the dislocation density increases, which in turn increases by plastically deforming the material.

The degree of plastic deformation can be expressed as *percent cold work* rather than strain:

$$\%CW = \frac{A_0 - A_d}{A_0} \times 100 \quad (43)$$

where A_0 is the original cross-sectional area and A_d is the cross-sectional area after deformation.

The relationship between yield strength and dislocation density can be derived starting with the relationship between yield strength and the applied resolved shear stress. The system with the largest resolved shear stress is favoured for slip to occur:

$$\tau_R = \sigma(\cos \lambda \cos \phi)_{\max} \quad (44)$$

Furthermore, for each material, there will be a critical value for τ_R known as the *critically resolved shear stress* at which slip will initiate. Therefore, a crystal will plastically deform when $\tau_R = \tau_{\text{CRSS}}$. Thus, noting that $\cos \lambda \cos \phi$ is at a max when $\lambda = \phi = 45^\circ$,

$$\tau_{\text{CRSS}} = \frac{1}{2} \sigma_y. \quad (45)$$

Pairing this with the empirically derived relationship

$$\tau_{\text{CRSS}} = \tau_0 + A\sqrt{\rho_\perp} \quad (46)$$

we can see that

$$\sigma_y \approx 2\tau_0 + 2A\sqrt{\rho_\perp}. \quad (47)$$

Or in other words, increasing ρ_\perp will lead to an increase in σ_y .

Q6.4 Precipitation strengthening

Precipitation strengthening involves second-phase particles (known as *precipitates*) being embedded in the host metal's matrix. These precipitates are much harder than the matrix itself, making it very difficult for a dislocation to shear through one.

When a dislocation encounters an embedded precipitate, one of two results may follow:

- If the plane of the precipitate is congruent with the plane of the matrix, or if the precipitate atoms are small, it is possible for the dislocation to shear through it. However this will require a large external shear stress, much larger than would be otherwise required. Hence the yield strength of the metal increases.
- More commonly, the dislocation is not able to pass through, with the precipitates acting as “pinning” sites, forming a Frank-Read-esk dislocation source. The dislocation line is forced to bend around these pins which requires extra external force, once again leading to an increase in the yield strength of the metal. If the distance between the pinning sites (the precipitates) is termed S , then

$$\sigma_y \propto \frac{1}{S} \quad (48)$$

Therefore, in either case, a larger force is required to deal with the embedded precipitates, increasing the yield strength of the metal.

Q6.5 FCC structures' larger ductility

The mechanism of slip and its consequences — namely, plastic deformation — have been thoroughly discussed so far. However, what is yet to be explained is *where* slip occurs in a crystal structure.

In any structure, there is always some preferred planes for dislocations to take place. These are known as the *slip planes*. Furthermore, in these planes, there are specific directions along which

dislocation motion occurs. These directions are known as *slip directions*. It so happens that the slip plane is the plane with the greatest atomic packing i.e. the plane with the greatest planar density. Similarly, the slip direction is the direction inside the slip plane with the greatest linear density. The combination of these slip planes and the slip directions is known as the *slip system*.

For example, in a face-centered cubic structure, the planes with the densest atomic packing (the close-packed planes) are the $\{111\}$ family (see Figure 7). Inside this plane, slip will occur in the directions with the greatest linear density, which are the $\langle 110 \rangle$ directions. Therefore, the entire slip system is represented by $\{111\}\langle 110 \rangle$.

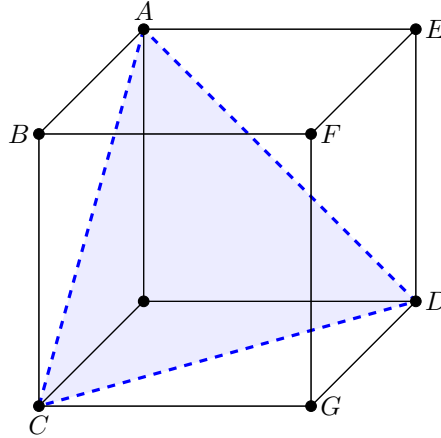


Figure 7: A close-packed plane in the FCC structure.

As ductility is a measure of how much plastic deformation a material can withstand, and plastic deformation is caused by slip, it is intuitive that greater ductility results from a greater number of slip systems. The total number of slip systems in a structure is the total combinations of planes and directions. For an FCC structure, there are four planes in the $\{111\}$ family and 3 directions in the $\langle 110 \rangle$ family, leading to $3 \times 4 = 12$ total systems. However, HCP structures only have a total of 3 slip systems. This leads to fewer locations or directions for plastic deformation to occur, resulting in HCP structures generally being less ductile and formable than FCC structures.

Question 7

Annealing of cold worked metals can lead to recovery, recrystallisation and grain growth. Please describe the three phenomena and explain the driving force of the phenomena. Also briefly mention how these phenomena affect the mechanical properties of the metals. [10%]

As explained in section 6.3, plastic deformation (cold work) affects many mechanical properties of a metal including the dislocation density and yield strength. It also affects physical properties such as electrical conductivity and corrosion resistance. Metals can be given an appropriate heat treatment (some treatment at an elevated temperature) in order to revert these properties back to the precold-worked states. This is known as *annealing*.

The main driving force for all three stages is the need to reduce the total system's energy.

Q7.1 Recovery

Some of the internal strain energy stored in the material's lattice is able to be relieved through enhanced atomic diffusion at elevated temperatures — atoms are able to diffuse to regions of tension or compression (around dislocations), therefore forming two dislocations of opposite sign which eventually undergo dislocation annihilation. Or, through the process of vacancy diffusion, the dislocations climb up in the lattice structure, meet an opposing dislocation and annihilate. If the dislocations are of the same sign, they arrange themselves in such a way as to reduce the overall lattice strain, and thus align themselves one on top of the other. Furthermore, point defects are annihilated to the surface or the grain boundaries and the point defect density decreases. Key to this stage is that no change to the grain structure occurs, and the only changes taking place are the dislocation arrangements in pre-existing grains. Often after this stage, some physical properties such as electrical and thermal conductivity return to their precold-worked states, and as recovery reduces the dislocation density, the process is normally accompanied by a reduction in a material's strength and a simultaneous increase in the ductility.

Q7.2 Recrystallisation

Even after the recovery stage, not all dislocations have disappeared. In fact, dislocation density remains relatively high and thus so does the total strain energy. This is the driving force for the phenomenon of recrystallisation: the difference in internal energy between the cold-worked and precold-worked materials. Recrystallisation describes the formation of a new set of strain-free grains with low dislocation densities which ultimately replace the deformed crystals. These new crystals are characteristic of the precold-worked material, and thus the mechanical properties are also restored i.e. the material becomes softer, weaker, and more ductile. The process involves new grains forming from small nuclei, which grow until they completely consume the parent material (the process ends when all cold-worked grains have been consumed).

We define the *recrystallisation temperature* T_R as the temperature at which recrystallisation is able to just complete in 1 hour. There are also a few other key variables which have an effect on the recrystallisation process:

1. Degree of prior deformation: the higher the percent cold work, the higher the amount of stored energy. This increases the driving force, enhancing the rate of recrystallisation and lowering the recrystallisation temperature. This effect reaches a limiting value at high deformations.

2. Initial grain size: the finer the initial grain size, the longer the total length of all grain boundaries. As these grain boundaries act as nucleation sites for the new grains, the rate of recrystallisation increases, and thus recrystallisation temperature will reduce.
3. Recrystallisation temperature: the recrystallisation rate depends exponentially on temperature, dictated by the following Arrhenius-esk equation:

$$\text{rate} = A \exp\left(-\frac{Q}{RT}\right) \quad (49)$$

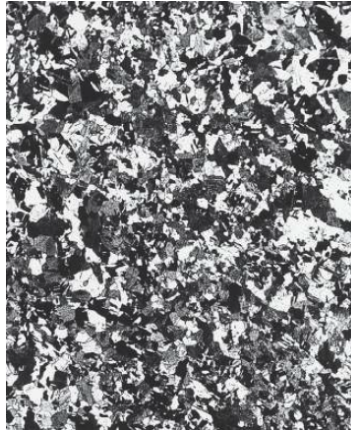


Figure 8: Complete recrystallisation of a cold-worked material.

Q7.3 Grain growth

Examine Figure 8, a photomicrograph of a material post-recrystallisation. At this moment, the total energy of the lattice is incredibly high and is in a “high-energy state” due to the small size and extreme number of grain boundaries (the crystallographic misorientation leads to a less efficient atomic packing, leading to a less ordered structure and higher internal energy). This is also known as the grain boundary surface energy. Therefore, in order to reduce the number of grain boundaries and their size, the phenomenon of ‘grain growth’ occurs — the increase in the average grain size of a material post-recrystallisation if left at the same temperature, resulting in a decrease in the total number of grains.

Grain growth occurs by the migration of grain boundaries; large grains grow at the expense of small ones which shrink. For many polycrystalline materials, the grain diameter d varies with t according to:

$$d^n - d_0^n = Kt \quad (50)$$

where d_0 is the initial grain diameter and K and n are constants.

We discussed in section 6.1 that *reducing* the grain size of a material leads to an increase in tensile strength, and reduction in ductility. Hence, post-grain *growth*, the material will experience a decrease in strength and increase in ductility.