# 计算物理模拟实验

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# 课程安排

第一学期　　2025年8月31日至2026年1月10日

| 周次 | 日 | 一 | 二 | 三 | 四 | 五 | 六 |
|---|---|---|---|---|---|---|---|
| 0 | 31 | 9/1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| 2 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| 3 | 21 | 22 | 23 | 24 | 25 | 26 | 27 |
| 4 | 28 | 29 | 30 | 10/1 | 2 | 3 | 4 |
| 5 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| 6 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
| 7 | 19 | 20 | 21 | 22 | 23 | 24 | 25 |
| 8 | 26 | 27 | 28 | 29 | 30 | 31 | 11/1 |
| 9 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| 10 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
| 11 | 16 | 17 | 18 | 19 | 20 | 21 | 22 |
| 12 | 23 | 24 | 25 | 26 | 27 | 28 | 29 |
| 13 | 30 | 12/1 | 2 | 3 | 4 | 5 | 6 |
| 14 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| 15 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| 16 | 21 | 22 | 23 | 24 | 25 | 26 | 27 |
| 17 | 28 | 29 | 30 | 31 | 1/1 | 2 | 3 |
| 18 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |

备　注

1. 2025级本科生8月31日报到，9月1日至9月5日入学教育，9月8日上课。
2. 2025级研究生9月1日报到，9月1日至9月5日入学教育，9月8日上课。
3. 本科生老生线上申请补考，9月3日至9月7日补考，9月7日注册，9月8日上课。
4. 研究生老生线上申请补考，9月3日至9月7日补考，9月5日注册，9月8日上课。
5. 2025级本科生、研究生开学典礼于第0周举行。
6. 中秋节、国庆节、元旦节放假以学校办通知为准。
7. 通识教育课程考试安排在第16周，第17、18周为停课考试周。
8. 第一学期于2026年1月10日结束，共计18教学周（包括考试）。

**时间：** 周六上午9点

**地点：** 江湾校区交叉一号楼A5005

Project 1 理论课

Project 1 进展总结

Project 1 汇报

Project 2 理论课

Project 2 进展总结

Project 2 汇报

其余时间每周六为答疑时间

# 课程考核

课题汇报（50%）

程序 +实验报告 (45% ）截止日期： 每次课题汇报后一周

课程反馈 （5%）

汇报和报告要求对于使用方法的讨论（包括但不限于计算效率/误差来源/局限性/改进方式），模拟的结果与绘图，实验内容的思考，参考文献等

**旨在借助计算模拟的方法去加深对物理学的重要知识点的理解，对编程技巧不做考核，鼓励使用AI，但注意AI可能会误导！**

写一个BFGS方法的晶格优化python程序

GPT-4-Turbo Poe ···

BFGS（Broyden-Fletcher-Goldfarb-Shanno）方法是一种在数值优化中广泛使用的拟牛顿方法，它用于寻找非线性优化问题的局部最优解。在材料科学和固体物理学中，BFGS方法常用于晶体结构的优化，即调整原子的位置以最小化系统的总能量。

下面，我将为你提供一个使用BFGS方法进行晶格优化的Python程序。这个例子将使用 `scipy.optimize.minimize`函数，它支持BFGS算法。我们将使用一个简单的势能模型（如Lennard-Jones势）来模拟原子间的相互作用，以此作为优化的目标函数。

**程序步骤**

1. **定义势能函数**：使用Lennard-Jones势来模拟两个原子间的相互作用。
2. **初始化原子位置**：设置初始的原子位置。
3. **优化过程**：使用BFGS算法优化原子位置。

**Python 代码实现**

python 复制

```python
import numpy as np
from scipy.optimize import minimize

def lennard_jones_potential(r):
    """
    Lennard-Jones potential function, where r is the distance between two atoms.
    """
    sigma = 1.0  # Characteristic length
    epsilon = 1.0  # Depth of the potential well
    return 4 * epsilon * ((sigma / r)**12 - (sigma / r)**6)
```

不适用 scipy库

GPT-4-Turbo Poe ···

如果需要实现BFGS方法而不使用scipy库，我们可以直接编写BFGS算法的相关代码。这会涉及到更多的数值计算细节，包括梯度的计算和BFGS更新公式的实现。以下是一个不使用scipy的BFGS方法的示例，该示例仍用于最小化Lennard-Jones势能函数。

**Python 代码实现**

python 复制

```python
import numpy as np

def lennard_jones_potential(r):
    sigma = 1.0
    epsilon = 1.0
    return 4 * epsilon * ((sigma / r)**12 - (sigma / r)**6)

def compute_gradients(positions):
    n_atoms = len(positions) // 3
    gradients = np.zeros_like(positions)
    for i in range(n_atoms):
```

# 晶体弹性模拟计算实验

## 实验目的

1. 了解固体力学性质和原子键合关系
2. 掌握弹性常数等力学量的计算方式
3. 理解弹性波在晶体中的传播
4. 认识温度对力学性能的影响

## 实验内容

基于原子间相互作用势编写程序计算模拟金属铝和绝缘体金刚石的零温和有限温下的力学性质。并思考分析以下问题：

1. 思考不同化学键对弹性常数以及物理性质的影响，分析计算误差来源与如何降低误差。探索不同晶系的独立矩阵元是否有不同。
2. 基于弹性常数计算两种体系的各种力学量和固体性质，模拟不同晶体中弹性波在[100]、[110]、[111]方向的传播，观察横波和纵波的区别。

3. 模拟不同的Strain大小对应的Stress， 得到Strain-Stress relation，思考在多大的范围内胡克定律成立？

4. 模拟金刚石不同温度下的弹性常数，观察不同弹性常数随温度变化的趋势。

# Elasticity

- Important because most engineering design is done in the elastic region. (Remember, plastic deformation generally constitutes failure.)
- Macroscopically, most polycrystalline materials are elastically isotropic.
- Microscopically, elastic behavior is inherently anisotropic for individual grains.
- Polycrystalline materials can be anisotropic if they exhibit strong crystallographic textures.

# Elasticity

- Derived from atomic bonding forces originating from long range attractive forces which draw atoms together until short range repulsive forces become large enough to balance them out.

- As such, elastic properties are an aggregate effect of individual deformations of interatomic bonds.

# Bulk Elastic Behavior

- Applied force is transmitted by the network of bonds constituting the material.
- Thus, elastic behavior depends quantitatively on the magnitude of the interatomic forces.
- Elastic properties <u>do not</u> depend on microstructure of the material.

# Forces Between Atoms

- Bonds form when atoms either share (e.g., covalent and metallic bonds) or transfer (e.g., ionic bonds) electrons between atoms.
- This occurs to achieve a minimum in potential energy for the system corresponding to a stable electron configuration.
- This has been modeled for ionic systems as follows:

# Ionic Bond

- Electron transfer from one atom to another occurs due to electrostatic interaction between oppositely charged ions (e.g., $Na^+$ and $Cl^-$ in NaCl).

- Force of attraction between ions is $F_{attract}$

$$F_{attract} = \frac{q^2}{4\pi\varepsilon_o r^2}$$

$q$ = charge of ion

$\varepsilon_o$ = permittivity of free space

$r$ = ionic separation distance

- Work is done to draw ions together. It is given by:

$$U_{attract} = \int_{\infty}^{r} F_{attract}\, dr = \frac{-q^2}{4\pi\varepsilon_o r} = \frac{-A}{r^m}$$

- Each atom maintains an electron cloud surrounding it. The outer surfaces of each atom are both negatively charged.

- Thus, at close distances, the electron clouds overlap and repel. The repulsive force can be written as:

$$U_{repel} = \frac{B}{r^n}$$

- The total energy of the system is thus the sum of the attractive and repulsive components. It can be expressed in general as:

$$U_{\text{total}} = U_{\text{attract}} + U_{\text{repel}} = \frac{-A}{r^m} + \frac{B}{r^n}$$

- This is the well known Lennard-Jones potential. You might recall this from your chemistry or physics courses.

- The minimum energy point corresponds to the equilibrium separation (i.e., the equilibrium bond length, $r_o$).

- The force between atoms is simply the derivative (i.e., the slope) of the energy versus distance plot.

$$F = \frac{-dU_{total}}{dr}$$

- The bond stiffness is the derivative of the force versus distance plot.

$$S = \frac{dF}{dr} = \frac{d^2U_{total}}{dr^2}$$

- At the equilibrium bond length, $r_o$, the variation of $F$ with $r$ is essentially linear, which means that the stiffness is essentially constant at small distances from $r_o$.

$$S_o = \left.\frac{dF}{dr}\right|_{r_o}$$

- Using this expression, the force to "stretch" $n$ bonds in a solid is:

$$F = n\int_{r_o}^{r} S_o dr = nS_o\left(r - r_o\right)$$

where $n$ is the number of bonds.

- The applied stress is:

$$\sigma = \frac{F}{A} = \frac{nS_o\left(r - r_o\right)}{nr_o^2}$$

- The strain can be expressed as:

$$\varepsilon = \frac{r - r_o}{r_o}$$

- Thus, stress becomes:

$$\sigma = \frac{F}{A} = \frac{nS_o(r - r_o)}{nr_o^2} = \frac{S_o}{r_o}\frac{(r - r_o)}{r_o} = \frac{S_o}{r_o}\varepsilon$$

- From Hooke's law:

$$\sigma = E\varepsilon$$

- Thus,

$$E = \frac{S_o}{r_o} = \frac{1}{r_o}\frac{d^2U}{dr^2}\bigg|_{r=r_o}$$

The derived expression shows that the modulus is dependent upon bonding.

Modulus, and other elastic properties, are <u>structure</u> <u>insensitive</u>.

The directionality of elastic properties <u>does</u> depend upon atomic arrangement (crystallography) in single crystals. They tend to average out in polycrystals.

| Bonding Type | Material, Substance | Bonding Energy | | Melting Temperature °C |
|---|---|---|---|---|
| | | kJ/mol | eV/Atom, Ion, Molecule | |
| Ionic | NaCl | 640 | 3.3 | 801 |
| | MgO | 1000 | 5.2 | 2800 |
| Covalent | Si | 450 | 4.7 | 1410 |
| | C (diamond) | 713 | 7.4 | >3550 |
| Metallic | Hg | 68 | 0.7 | -39 |
| | Al | 324 | 3.4 | 660 |
| | Fe | 406 | 4.2 | 1538 |
| | W | 849 | 8.8 | 3410 |
| van der Waals | Ar | 7.7 | 0.08 | -189 |
| | $Cl_2$ | 31 | 0.32 | -101 |
| Hydrogen | $NH_3$ | 35 | 0.36 | -78 |
| | $H_2O$ | 51 | 0.52 | 0 |

[From W.D. Callister, Jr, Materials Science and Engineering: An Introduction, 7th Ed., (Wiley, New York, 2007) p.28]

Ceramics
Tungsten carbides
Silicon carbide
Tungsten alloys
Aluminum nitride
Cast iron, ductile (nodular)
Metals
Zinc alloys
Tin
Aluminum alloys
Titanium alloys
Magnesium alloys
Lead alloys
Brick
Stone
Ceramics
Concrete
Polyethylene terephthalate (PET)
Polyurethane (tpPUR)
Polyamides (Nylons, PA)
Polymers
Polypropylene (PP)
Polyethylene (PE)
Polytetrafluoroethylene (Teflon, PTFE)
Ionomer (I)
Young's modulus (GPa)
1000
100
10
1
0.1
100
200
500
1000
2000
Melting point (°C)

Courtesy of Granta Design

A bar chart illustrating Young's moduli for some common examples of the primary classes of materials (i.e., metals, ceramics, polymers and composites). Ceramics tend to exhibit the highest elastic moduli and polymers the lowest. The elastic moduli of composites are between those of their constituents.

# stress is related to strain for an isotropic solid

Stress-strain plot for a linearly elastic material

- Hooke's Law
  - Isotropic Solids (properties are the same in all directions)

$$\sigma = \varepsilon E \text{ or } \varepsilon = \frac{1}{E}\sigma$$

  - Anisotropic solids (properties are directional)

Need different definition

  - Let's consider both cases

# First consider the Poisson effect

$$\nu(z,x) = -\frac{\varepsilon_x}{\varepsilon_z} \quad \text{and} \quad \nu(z,y) = -\frac{\varepsilon_y}{\varepsilon_z}$$

A tensile stress along the *z* axis causes the material to stretch along the *z* axis and to contract along the *x* and *y* axes.

$$\text{Poisson's Ratio, } \nu = -\frac{\text{lateral strain}}{\text{longitudinal strain}}$$

## Room- Temperature Poisson's Ratio for Selected Solids

| Material Class | Material | $\nu$ |
|---|---|---|
| Metallic solid (crystalline) | Ag | 0.38 |
| | Al | 0.34 |
| | Au | 0.42 |
| | Cu | 0.34 |
| | $\alpha$-Fe | 0.29 |
| | Ir | 0.26 |
| | Ni | 0.31 |
| | W | 0.29 |
| Covalent solid (crystalline) | Ge | 0.28 |
| | Si | 0.27 |
| | $Al_2O_3$ | 0.23 |
| | TiC | 0.19 |
| Covalent Ionic Solid | MgO | 0.19 |
| Covalent Glass | Silica glass | 0.20 |
| Network Polymer | Bakelite | 0.20 |
| | Ebonite (hard rubber) | 0.39 |
| Elastomer | Natural rubber | 0.49 |
| Chain Polymer | Polystyrene | 0.33 |
| | Polyethylene | 0.40 |
| Van der Waal's Solid | Argon (at 0 K) | 0.25 |

The strains resulting from this stress state must be the sum of the strains associated with loading along each individual axis.

$$\mathrm{B}:\ \varepsilon_{xx}^{\mathrm{B}} = \frac{\sigma_{xx}}{E},\quad \varepsilon_{yy}^{\mathrm{B}} = -\nu\varepsilon_{xx}^{\mathrm{B}} = -\nu\frac{\sigma_{xx}}{E}$$

$$\mathrm{C}:\ \varepsilon_{yy}^{\mathrm{C}} = \frac{\sigma_{yy}}{E},\quad \varepsilon_{xx}^{\mathrm{C}} = -\nu\varepsilon_{yy}^{\mathrm{C}} = -\nu\frac{\sigma_{yy}}{E}$$

$$\mathrm{A}=\mathrm{B}+\mathrm{C}:\ \varepsilon_{xx} = \varepsilon_{xx}^{\mathrm{B}} + \varepsilon_{xx}^{\mathrm{C}} = \frac{\sigma_{xx}}{E} - \nu\frac{\sigma_{yy}}{E}$$

(There's a similar expression for $\varepsilon_{yy}$)

# Elastic Stress-Strain Relations

| Stress | Strain in the x-direction | Strain in the y-direction | Strain in the z-direction |
|---|---|---|---|
| $\sigma_{xx} \longrightarrow$ | $\varepsilon_{xx} = \dfrac{\sigma_{xx}}{E}$ | $\varepsilon_{yy} = -\dfrac{\nu\sigma_{xx}}{E}$ | $\varepsilon_{zz} = -\dfrac{\nu\sigma_{xx}}{E}$ |
| $\sigma_{yy} \longrightarrow$ | $\varepsilon_{xx} = -\dfrac{\nu\sigma_{yy}}{E}$ | $\varepsilon_{yy} = \dfrac{\sigma_{yy}}{E}$ | $\varepsilon_{zz} = -\dfrac{\nu\sigma_{yy}}{E}$ |
| $\sigma_{zz} \longrightarrow$ | $\varepsilon_{xx} = -\dfrac{\nu\sigma_{zz}}{E}$ | $\varepsilon_{yy} = -\dfrac{\nu\sigma_{zz}}{E}$ | $\varepsilon_{zz} = \dfrac{\sigma_{zz}}{E}$ |

$$\boldsymbol{\varepsilon}_{xx} = \frac{1}{E}\left[\boldsymbol{\sigma}_{xx} - \boldsymbol{\nu}\left(\boldsymbol{\sigma}_{yy} + \boldsymbol{\sigma}_{zz}\right)\right]$$

$$\boldsymbol{\varepsilon}_{yy} = \frac{1}{E}\left[\boldsymbol{\sigma}_{yy} - \boldsymbol{\nu}\left(\boldsymbol{\sigma}_{zz} + \boldsymbol{\sigma}_{xx}\right)\right]$$

$$\boldsymbol{\varepsilon}_{zz} = \frac{1}{E}\left[\boldsymbol{\sigma}_{zz} - \boldsymbol{\nu}\left(\boldsymbol{\sigma}_{xx} + \boldsymbol{\sigma}_{yy}\right)\right]$$

$$\tau_{xy} = G\gamma_{xy};\ \tau_{yz} = G\gamma_{yz};\ \tau_{xz} = G\gamma_{xz}$$

Variation in elastic strain for an **isotropic solid** because of the Poisson effect

# Other Elastic Stress-Strain Relations for Isotropic Solid

- Bulk Modulus ($K$), also known as the *volumetric elastic modulus*:

$$K = \frac{\text{hydrostatic pressure}}{\text{volume change produced}} = \frac{\sigma_m}{\Delta} = \frac{-p}{\Delta} = \frac{1}{B}$$

where:

$$-p = \text{hydrostatic pressure},$$

$$\sigma_m = \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3}$$

$$\Delta = \text{dilatation (i.e., volume change)} = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz},$$

$$B = \text{compressibility.}$$

# Other Elastic Stress-Strain Relations for Isotropic Solid

- Now we can relate the elastic constants.

$$\boldsymbol{\varepsilon}_{xx} = \frac{1}{E}\left[\boldsymbol{\sigma}_{xx} - \boldsymbol{\nu}\left(\boldsymbol{\sigma}_{yy} + \boldsymbol{\sigma}_{zz}\right)\right]$$

$$\boldsymbol{\varepsilon}_{yy} = \frac{1}{E}\left[\boldsymbol{\sigma}_{yy} - \boldsymbol{\nu}\left(\boldsymbol{\sigma}_{zz} + \boldsymbol{\sigma}_{xx}\right)\right]$$

$$\boldsymbol{\varepsilon}_{zz} = \frac{1}{E}\left[\boldsymbol{\sigma}_{zz} - \boldsymbol{\nu}\left(\boldsymbol{\sigma}_{xx} + \boldsymbol{\sigma}_{yy}\right)\right]$$

Summation yields:

$$\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} = \frac{1-2\nu}{E}\left(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}\right) = \frac{1-2\nu}{E}3\sigma_m = \Delta$$

$$\therefore \quad K = \frac{\sigma_m}{\Delta} = \frac{E}{3(1-2\nu)}$$

# Other Elastic Stress-Strain Relations for Isotropic Solid

| In terms / Elastic constants | $E, \nu$ | $E, G$ | $K, \nu$ | $E, G$ | $\lambda, \mu$ |
|---|---|---|---|---|---|
| $E$ [elastic] | $= E$ | $= E$ | $= 3(1-2\nu)K$ | $= \dfrac{9K}{1+3K/G}$ | $= \dfrac{\mu(3+2\mu/\lambda)}{2(1+\mu/\lambda)}$ |
| $\nu$ | $= \nu$ | $= -1+\dfrac{E}{2G}$ | $= \nu$ | $= \dfrac{1-2G/3K}{2+2G/3K}$ | $= \dfrac{1}{2(1+\mu/\lambda)}$ |
| $G$ [shear] | $= \dfrac{E}{2(1+\nu)}$ | $= G$ | $= \dfrac{3(1-2\nu)K}{2(1+\nu)}$ | $= G$ | $= \mu$ |
| $K$ [bulk] | $= \dfrac{E}{3(1-2\nu)}$ | $= \dfrac{E}{9-3E/G}$ | $= K$ | $= K$ | $= \lambda + \dfrac{2\mu}{3}$ |
| $\lambda$ | $= \dfrac{E\nu}{(1+\nu)(1-2\nu)}$ | $= \dfrac{E(1-2G/E)}{3-E/G}$ | $= \dfrac{3K\nu}{1+\nu}$ | $= K - \dfrac{2G}{3}$ | $= \lambda$ |
| $\mu$ | $= \dfrac{E}{2(1+\nu)}$ | $= G$ | $= \dfrac{3(1-2\nu)K}{2(1+\nu)}$ | $= G$ | $= \mu$ |

$\lambda, \mu$ = Lame constants

# Elastic Strain Energy

*Energy stored in a body due to deformation.*

- Work to deform a body elastically is stored as <u>elastic</u> <u>strain energy</u>. It is recovered when the applied forces are released.

- Strain energy is proportional to the area under the load-deformation (stress-strain) curve.

- We will elaborate on this concept on the next few pages.

# Elastic Strain Energy

- The first law of thermodynamics states:

  $$dU = \delta Q + \delta W = TdS - PdV$$

  where,

  $dU$ = internal energy
  $\delta Q$ = heat
  $\delta W$ = mechanical work done

- <u>During</u> <u>elastic</u> <u>deformation</u>, the amount of heat generated is negligible.

- Thus the work done on the body is converted into internal energy and is fully recovered upon unloading.

# Elastic Strain Energy

- Consider an elemental cube that is subjected to only an elastic tensile stress along the *x*-axis. The elastic strain energy, *U*, is:

$$U = \frac{1}{2}(\text{load})(\text{deformation})$$

$$\sigma_{xx} = \frac{F}{A}$$

$$\varepsilon_{xx} = \frac{du}{dx}$$

$$dU = \frac{1}{2}Fdu = \frac{1}{2}(\sigma_{xx}A)(\varepsilon_{xx}dx) = \frac{1}{2}(\sigma_{xx}\varepsilon_{xx})(Adx)$$

= total elastic energy absorbed by the material element.

Since *Adx* is the volume, the elastic strain energy per unit volume (i.e., the strain energy density) is:

$$U_o = \frac{dU}{Adx} = \frac{1}{2}(\sigma_{xx}\varepsilon_{xx}).$$

# Elastic Strain Energy

$$\sigma_{xx} = \frac{F}{A}$$

$$\varepsilon_{xx} = \frac{du}{dx}$$

From Hooke's law, $\varepsilon_{xx} = \dfrac{\sigma_{xx}}{E}$

Therefore:

$$U_o = \frac{1}{2}\frac{\sigma_{xx}^2}{E} = \frac{1}{2}\varepsilon_{xx}^2 E \text{ [in tension]}$$

$$U_o = \frac{1}{2}\left(\tau_{xy}\gamma_{xy}\right) = \frac{1}{2}\frac{\tau_{xy}^2}{G} = \frac{1}{2}\gamma_{xy}^2 G \text{ [in pure shear]}$$

In three dimensions, the general expression for elastic strain energy is:

$$U_o = \frac{1}{2}\left(\sigma_{xx}\varepsilon_{xx} + \sigma_{yy}\varepsilon_{yy} + \sigma_{zz}\varepsilon_{zz} + \tau_{xy}\gamma_{xy} + \tau_{xz}\gamma_{xz} + \tau_{yz}\gamma_{yz}\right).$$

# Elastic Strain Energy

In tensor notation, these general expressions become:

$$U_o = \frac{1}{2}\sigma_{ij}\varepsilon_{ij} = \frac{1}{2}\frac{\sigma_{ij}^2}{E} = \frac{1}{2}\varepsilon_{ij}^2 E.$$

If we substite into these expressions, the variation in elastic strain for an isotropic solid, accounting for the Poisson effect, we get:

$$U_o = \frac{1}{2E}\left(\sigma_{xx}^2 + \sigma_{yy}^2 + \sigma_{zz}^2\right) - \frac{\nu}{E}\left(\sigma_{xx}\sigma_{yy} + \sigma_{yy}\sigma_{zz} + \sigma_{xx}\sigma_{zz}\right) + \frac{1}{2G}\left(\tau_{xy}^2 + \tau_{xz}^2 + \tau_{yz}^2\right)$$

[for a 3D isotropic solid]

Expressed in terms of strains and elastic constants:

$$U_o = \frac{1}{2}\lambda\Delta^2 + G\left(\varepsilon_{xx}^2 + \varepsilon_{yy}^2 + \varepsilon_{zz}^2\right) + \frac{1}{2}G\left(\gamma_{xy}^2 + \gamma_{xz}^2 + \gamma_{yz}^2\right)$$

# Elastic Strain Energy

$$U_o = \frac{1}{2}\left(\sigma_{xx}\varepsilon_{xx} + \sigma_{yy}\varepsilon_{yy} + \sigma_{zz}\varepsilon_{zz} + \tau_{xy}\gamma_{xy} + \tau_{xz}\gamma_{xz} + \tau_{yz}\gamma_{yz}\right)$$

The derivative of $U_o$ with respect to any strain component yields the corresponding stress component, or:

$$\frac{\partial U_o}{\partial \varepsilon_{ij}} = \lambda\Delta + 2G\varepsilon_{ij} = \sigma_{ij}$$

Similarly, the derivative of $U_o$ with respect to any stress component yields the corresponding strain or:

$$\frac{\partial U_o}{\partial \sigma_{ij}} = \varepsilon_{ij}$$

You can use these terms to calculate stresses and strains in elasticty. Techniques for doing this include Castigliano's theorem, the theorem of least work, and the principal of virtual work.

# Anisotropy and Single Crystals

- Forces between atoms are directional.

- They act along the “lines” connecting the atoms together.

# Relations between stress and strain for anisotropic crystals

- Since force varies with direction, elastic constants will also vary.
- In general, we need to relate every stress component to every strain component.
- Thus we must define two new elastic constants:
  - $C \equiv$ stiffness
  - $S \equiv$ compliance
- We also re-write Hooke's law as:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \quad \text{or} \quad \varepsilon_{ij} = S_{ijkl}\sigma_{kl}$$

**Stiffness is a**
**4th rank tensor**
**$3^4 = 81$ terms**

$$\sigma_{ij} = \sum_{k=1}^{3}\sum_{l=1}^{3} C_{ijkl}\varepsilon_{kl}$$

$$\downarrow$$

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$$

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \\ \sigma_{zy} \\ \sigma_{xz} \\ \sigma_{yx} \end{pmatrix} = \begin{pmatrix} C_{xxxx} & C_{xxyy} & C_{xxzz} & C_{xxyz} & C_{xxzx} & C_{xxxy} & C_{xxzy} & C_{xxxz} & C_{xxyx} \\ C_{yyxx} & C_{yyyy} & C_{yyzz} & C_{yyyz} & C_{yyxz} & C_{yyxy} & C_{yyzy} & C_{yyxz} & C_{yyyx} \\ C_{zzxx} & C_{zzyy} & C_{zzzz} & C_{zzyz} & C_{zzxz} & C_{zzxy} & C_{zzzy} & C_{zzxz} & C_{zzyx} \\ C_{yzxx} & C_{yzyy} & C_{yzzz} & C_{yzyz} & C_{yzxz} & C_{yzxy} & C_{yzzy} & C_{yzxz} & C_{yzyx} \\ C_{zxxx} & C_{zxyy} & C_{zxzz} & C_{zxyz} & C_{zxxz} & C_{zxxy} & C_{zxzy} & C_{zxxz} & C_{zxyx} \\ C_{xyxx} & C_{xyyy} & C_{xyzz} & C_{xyyz} & C_{xyxz} & C_{xyxy} & C_{xyzy} & C_{xyxz} & C_{xyyx} \\ C_{zyxx} & C_{zyyy} & C_{zyzz} & C_{zyyz} & C_{zyxz} & C_{zyxy} & C_{zyzy} & C_{zyxz} & C_{zyyx} \\ C_{xzxx} & C_{xzyy} & C_{xzzz} & C_{xzyz} & C_{xzxz} & C_{xzxy} & C_{xzzy} & C_{xzxz} & C_{xzyx} \\ C_{yxxx} & C_{yxyy} & C_{yxzz} & C_{yxyz} & C_{yxxz} & C_{yxxy} & C_{yxzy} & C_{yxxz} & C_{yxyx} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \\ \varepsilon_{zy} \\ \varepsilon_{xz} \\ \varepsilon_{yx} \end{pmatrix}$$

Stress tensor

Elastic Stiffness

Strain tensor

$X_x$ is a force applied in the x direction to a unit area of a plane whose normal lies in the x direction; $X_y$ is applied in the x direction to a unit area of a plane whose normal lies in the y direction

The total torque about the origin is also zero if $Y_x$=$X_y$.

$$Y_z = Z_y \;; \qquad Z_x = X_z \;; \qquad X_y = Y_x$$

# EQUILIBRIUM CONSIDERATIONS

$$\sigma_{ij} = \sigma_{ji} \qquad \varepsilon_{kl} = \varepsilon_{lk}$$

$$C_{ijkl} = C_{jikl} \qquad C_{ijkl} = C_{jikl}$$

$$C_{ijkl} = C_{jikl} \qquad C_{ijkl} = C_{ijlk}$$

**Allow us to reduce the number of constants from 81 to 36**

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix} = \begin{pmatrix} C_{xxxx} & C_{xxyy} & C_{xxzz} & C_{xxyz} & C_{xxxz} & C_{xxxy} \\ C_{yyxx} & C_{yyyy} & C_{yyzz} & C_{yyyz} & C_{yyxz} & C_{yyxy} \\ C_{zzxx} & C_{zzyy} & C_{zzzz} & C_{zzyz} & C_{zzxz} & C_{zzxy} \\ C_{yzxx} & C_{yzyy} & C_{yzzz} & C_{yzyz} & C_{yzxz} & C_{yzxy} \\ C_{xzxx} & C_{xzyy} & C_{xzzz} & C_{xzyz} & C_{xzxz} & C_{xzxy} \\ C_{xyxx} & C_{xyyy} & C_{xyzz} & C_{xyyz} & C_{xyxz} & C_{xyxy} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{pmatrix}$$

$(\sigma_{xx})$

$$\begin{pmatrix} \sigma_{xz} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix} = \begin{pmatrix} C_{xxxx} & C_{xxyy} & C_{xxzz} & C_{xxyz} & C_{xxxz} & C_{xxxy} \\ C_{yyxx} & C_{yyyy} & C_{yyzz} & C_{yyyz} & C_{yyxz} & C_{yyxy} \\ C_{zzxx} & C_{zzyy} & C_{zzzz} & C_{zzyz} & C_{zzxz} & C_{zzxy} \\ C_{yzxx} & C_{yzyy} & C_{yzzz} & C_{yzyz} & C_{yzxz} & C_{yzxy} \\ C_{xzxx} & C_{xzyy} & C_{xzzz} & C_{xzyz} & C_{xzxz} & C_{xzxy} \\ C_{xyxx} & C_{xyyy} & C_{xyzz} & C_{xyyz} & C_{xyxz} & C_{xyxy} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{pmatrix}$$

$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \longrightarrow$ $C_{ijkl}$ is the STIFNESS matrix

$$\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{pmatrix} = \begin{pmatrix} S_{xxxx} & S_{xxyy} & S_{xxzz} & S_{xxyz} & S_{xxxz} & S_{xxxy} \\ S_{yyxx} & S_{yyyy} & S_{yyzz} & S_{yyyz} & S_{yyxz} & S_{yyxy} \\ S_{zzxx} & S_{zzyy} & S_{zzzz} & S_{zzyz} & S_{zzxz} & S_{zzxy} \\ S_{yzxx} & S_{yzyy} & S_{yzzz} & S_{yzyz} & S_{yzxz} & S_{yzxy} \\ S_{xzxx} & S_{xzyy} & S_{xzzz} & S_{xzyz} & S_{xzxz} & S_{xzxy} \\ S_{xyxx} & S_{xyyy} & S_{xyzz} & S_{xyyz} & S_{xyxz} & S_{xyxy} \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix}$$

$\varepsilon_{ij} = S_{ijkl}\sigma_{kl} \longrightarrow$ $S_{ijkl}$ is the COMPLIANCE matrix

# Matrix/Contracted Notation

- We often replace the indices with matrix (contracted) notation for simplicity [Voigt, <u>Lehrbuch der Kristallphysik</u> (Teubner VErlag, Berlin, 1910)].

$$xx \to 11 \to 1 \qquad yy \to 22 \to 2 \qquad zz \to 33 \to 3$$

$$yz \to 23 \to 4 \qquad xz \to 13 \to 5 \qquad xy \to 12 \to 6$$

$$\begin{pmatrix} 11 & 12 & 13 \\ & 22 & 23 \\ & & 33 \end{pmatrix} \equiv \begin{pmatrix} 1 & 6 & 5 \\ & 2 & 4 \\ & & 3 \end{pmatrix}$$

- Thus, Hooke's law is often re-written in matrix form as:

$$\sigma_p = C_{pq}\varepsilon_q \quad \text{or} \quad \varepsilon_p = S_{pq}\sigma_q$$

row column

# Additional note about contracted notation

- Numbers 1-3 are associated with normal stresses and strains.
- Numbers 4-6 are associated with shear stresses and strains.
- On the next slide I attempt to show you which stresses and strains are related to each elastic constant.

TENSOR

$$
\begin{array}{c}
\sigma,\varepsilon \qquad\qquad\qquad \sigma,\gamma \\
C_{ijkl} = \left(\begin{array}{ccc|ccc}
C_{xxxx} & C_{xxyy} & C_{xxzz} & C_{xxyz} & C_{xxxz} & C_{xxxy} \\
C_{yyxx} & C_{yyyy} & C_{yyzz} & C_{yyyz} & C_{yyxz} & C_{yyxy} \\
C_{zzxx} & C_{zzyy} & C_{zzzz} & C_{zzyz} & C_{zzxz} & C_{zzxy} \\
\hline
C_{yzxx} & C_{yzyy} & C_{yzzz} & C_{yzyz} & C_{yzxz} & C_{yzxy} \\
C_{xzxx} & C_{xzyy} & C_{xzzz} & C_{xzyz} & C_{xzxz} & C_{xzxy} \\
C_{xyxx} & C_{xyyy} & C_{xyzz} & C_{xyyz} & C_{xyxz} & C_{xyxy}
\end{array}\right) \\
\tau,\varepsilon \qquad\qquad\qquad \tau,\gamma
\end{array}
$$

---

CONTRACTED

$$
\begin{array}{c}
\sigma,\varepsilon \qquad\qquad\qquad \sigma,\gamma \\
C_{ijkl} = \left(\begin{array}{ccc|ccc}
C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\
\hline
C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\
C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\
C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66}
\end{array}\right) \\
\tau,\varepsilon \qquad\qquad\qquad \tau,\gamma
\end{array}
$$

# Contracted vs. Tensor Notation

- Contracted notation is simple and convenient for conducting matrix inversions.

► However, for coordinate transformations or invariant determination, it is more useful to use the stiffness and compliances in tensor notation.

*Note the change from tensor notation to matrix notation. See Chapter 8 in Nye for details.*

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix}$$

$\sigma_p = C_{pq}\varepsilon_q \longrightarrow$ $C_{pq}$ is the STIFNESS matrix

$$\begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{21} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{31} & S_{32} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{41} & S_{42} & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & S_{53} & S_{54} & S_{55} & S_{56} \\ S_{61} & S_{62} & S_{63} & S_{64} & S_{65} & S_{66} \end{pmatrix} \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix}$$

$\varepsilon_p = S_{pq}\sigma_q \longrightarrow$ $S_{pq}$ is the COMPLIANCE matrix

Stiffness and compliance matrices are also symmetric about the main diagonal

$$\begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{pmatrix} \rightarrow \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ \cdot & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ \cdot & \cdot & C_{33} & C_{34} & C_{35} & C_{36} \\ \cdot & \cdot & \cdot & C_{44} & C_{45} & C_{46} \\ \cdot & \cdot & \cdot & \cdot & C_{55} & C_{56} \\ \cdot & \cdot & \cdot & \cdot & \cdot & C_{66} \end{pmatrix}$$

$$\begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{21} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{31} & S_{32} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{41} & S_{42} & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & S_{53} & S_{54} & S_{55} & S_{56} \\ S_{61} & S_{62} & S_{63} & S_{64} & S_{65} & S_{66} \end{pmatrix} \rightarrow \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ \cdot & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ \cdot & \cdot & S_{33} & S_{34} & S_{35} & S_{36} \\ \cdot & \cdot & \cdot & S_{44} & S_{45} & S_{46} \\ \cdot & \cdot & \cdot & \cdot & S_{55} & S_{56} \\ \cdot & \cdot & \cdot & \cdot & \cdot & S_{66} \end{pmatrix}$$

Required number of components reduces to 21

The number can be further reduced by considering crystal symmetry

# Neumann's Principle

- “The symmetry of any physical property of a crystal must include the symmetry elements of the point group of the crystal.”

- Point groups are the group of macroscopic symmetry elements possessed by the structure of a crystal.*

- Crystals exhibit specific point symmetries.

- Crystal “properties” will include the point group but can exhibit more symmetry than the point group.

* Review pages 20-25 and 279-288 in Nye for a more complete treatment.

# Possible Macroscopic Symmetry Elements

- Center of symmetry
- Mirror plane
- ► 1-, 2-, 3-, 4- or 6-fold rotation axes
- 1-, 2-, 3-, 4- or 6-fold inversion axes

## Crystal systems

- The 32 crystal classes (i.e., point groups) are conventionally grouped into seven crystal systems.
- The requirements for membership in a given crystal system is that the symmetry of the class should possess a certain minimum characteristic.

Symbolism for the symmetry elements of the 32 point groups

| *Symmetry element* | *Symbol on stereogram* | *International symbol* |
|---|---|---|
| centre of symmetry | no symbol | $\bar{1}$ |
| mirror plane | full line (great circle) | $m$ |
| *Rotation axes* | | |
| 1-fold (monad) | no symbol | $1$ |
| 2-fold (diad) | | $2$ |
| 3-fold (triad) | | $3$ |
| 4-fold (tetrad) | | $4$ |
| 6-fold (hexad) | | $6$ |
| *Inversion axes* | | |
| 1-fold (inverse monad) ≡ centre of symmetry | no symbol | $\bar{1}$ |
| 2-fold (inverse diad) ≡ mirror plane normal to the axis | as for mirror plane | $\bar{2}$ (≡ $m$) |
| 3-fold (inverse triad) ≡ 3-fold rotation axis plus a centre of symmetry | | $\bar{3}$ |
| 4-fold (inverse tetrad) (includes a rotation diad axis) | | $\bar{4}$ |
| 6-fold (inverse hexad) ≡ a rotation triad axis plus a plane normal to it | | $\bar{6}$ (≡ $3/m$) |

[Table from J.F. Nye, Physical Properties of Crystals, (Oxford University Press, Oxford, 1985) p. 280]

- We can describe shapes and arrangements of points within shapes in terms of the symmetry exhibited by them.

- In crystal systems, the symmetry of a class of crystals should possess a certain characteristic symmetry (i.e., certain minimum symmetry elements).

## We describe crystal symmetry relative to specific crystallographic axes and symmetry elements operating on those axes

The order of Hermann-Mauguin symbols in point groups

| Crystal System | Primary | Secondary | Tertiary |
|---|---|---|---|
| Triclinic | – | – | – |
| Monoclinic | [010], unique axis b<br>[001], unique axis c | – | – |
| Orthorhombic | [100] | [010] | [001] |
| Tetragonal | [001] | [100], [010] | $[1\bar{1}0]$, [110] |
| Trigonal, Rhombohedral Axes | [111] | $[1\bar{1}0]$, $[01\bar{1}]$, $[\bar{1}01]$ | |
| Trigonal, Hexagonal Axes | [001] | [100], [010], $[\bar{1}\bar{1}0]$ | |
| Hexagonal | [001] | [100], [010], $[\bar{1}\bar{1}0]$ | $[1\bar{1}0]$, [120, $[\bar{2}\bar{1}0]$ |
| Cubic | [100], [010], [001] | [111], $[1\bar{1}\bar{1}]$, $[\bar{1}1\bar{1}]$, $[\bar{1}\bar{1}1]$ | $[1\bar{1}0]$, [110], $[01\bar{1}]$,<br>[011], $[\bar{1}01]$, [101] |

Table adapted from R. Tilley, *Crystals and Crystal Structures*, John Wiley & Sons, Hoboken, NJ, 2006, p. 73.

**The concept of crystal symmetry is illustrated on the next six viewgraphs.**

**You should review this and related literature on your own time.**

- Rotation about the center point.
- 180° rotation moves point “1” to “2” but produces same pattern.
- Second 180° rotation moves original point (labeled with a “1”) back to its starting point.
- 2-fold rotation.

# $\bar{4}3m$

Tetrahedron inscribed in a cube

4-fold inversion axes parallel to x,y,z (aka, <100>)

3-fold rotation axes parallel to cube diagonals (aka, <111>)

Mirror plane parallel to face diagonals (aka, <110>)

Symmetry elements in a regular tetrahedron. (a) tetrahedron inscribed in a cube showing three Cartesian axes; (b) 4-fold inversion axes along *x* [100], *y* [010] and *z* [001]; (c) 3-fold rotation axes passing through vertex and center of opposite triangular face (i.e., [111]); (d) mirror planes parallel to [110]. Adapted from Fig. 4.6 in R. Tilley, *Crystals and Crystal Structures*, John Wiley & Sons, Hoboken, NJ, 2006.

# $4\bar{3}m$

Octahedron inscribed in a cube

4-fold rotation axes parallel to x,y,z (aka, <100>) with perpendicular mirror plane.

3-fold inversion axes parallel to cube diagonals (aka, <111>)

2-fold rotation axes parallel to face diagonals (aka, <111>) with perpendicular mirror plane.

R. Tilley, *Crystals and Crystal Structures*, John Wiley & Sons, Hoboken, NJ, 2006.

**Figure 4.7** Symmetry elements present in a regular octahedron: (a) an octahedron in a cube, showing the three Cartesian axes; (b) each tetrad rotation axis (4) lies along either x-, y- or z and is normal to a mirror plane; (c) three-fold inversion axes ($\bar{3}$) pass through the centre of each triangular face; (d) a triangular face viewed from above; (d) diad axes through the centre of each edge lie normal to mirror planes

We describe lattice shapes and arrangements of lattice points in the same way.

# Symmetry of the Cubic P-Lattice

**Primary** **Secondary** **Tertiary**

**Four 3-fold rotation axes parallel to cube diagonals (aka, <111>)**

**Fig. 6.24.** a Space group P 4/m 3̄ 2/m . In the other diagrams, only the symmetry elements corresponding to the symmetry directions ⟨a⟩, ⟨111⟩, ⟨110⟩ are shown.
**b** P 4/m . . . ., **c** P . . . 3̄ . . ., **d** P . . . . 2/m
↓ ⟨a⟩ ↓ ⟨111⟩ ↓ ⟨110⟩

Adapted from W. Borchardt-Ott, *Crystallography, 2nd Edition*, (Springer, Berlin, Germany, 1995) p. 99

- There are only 32 crystal classes derived from the 7 crystal systems (i.e., shapes).
- Each has a certain characteristic symmetry.
- They are presented on stereograms on this viewgraph and the two that follow.

**Table 21**

***Symmetry elements and conventions for the choice of axes in the 32 crystal classes***

Symbols of centrosymmetrical classes are enclosed in boxes

[Nye, p. 284]

Table 21.3

## Tetragonal

Table 21.2

[Nye, pp. 285-286]

## Trigonal

Table 21.3

**Hexagonal**

[Nye, pp. 287-288]

Table 21.4

**Cubic**

Table 21.5

# Influence of Crystal Symmetry on Number of Elastic Constants

| Crystal System | Axial Relation-ships | Interaxial Angles | Minimum Symmetry Elements | Number of Elastic Constants |
|---|---|---|---|---|
| **Cubic** | $a = b = c$ | $\alpha = \beta = \gamma = 90°$ | **Four 3-fold rotation** or rotoinversion axes parallel to body diagonals | 3 |
| **Hexagonal** | $a = b \neq c$ | $\alpha = \beta = 90°$; $\gamma = 120°$ | **One 6-fold rotation** or rotoinversion axis parallel to *z*-axis | 5 |
| **Tetragonal** | $a = b \neq c$ | $\alpha = \beta = \gamma = 90°$ | **One 4-fold rotation** or rotoinversion axis parallel to *z*-axis | 6 or 7 |
| **Rhombohedral (Trigonal)** | $a = b = c$ | $\alpha = \beta = \gamma \neq 90°$ | **One 3-fold rotation** or rotoinversion axis parallel to *z*-axis | 5, 6 or 7 |
| **Orthorhombic** | $a \neq b \neq c$ | $\alpha = \beta = \gamma = 90°$ | **Three 2-fold rotation** or rotoinversion axes parallel to *x*,*y*,*z*-axes | 9 |
| **Monoclinic** | $a \neq b \neq c$ | $\alpha = \gamma = 90° \neq \beta$ | **One 2-fold rotation** or rotoinversion axis parallel to *y*-axis | 13 |
| **Triclinic** | $a \neq b \neq c$ | $\alpha \neq \beta \neq \gamma \neq 90°$ | - None - **One 1-fold rotation** or rotoinversion axis | 21 |

Increasing crystal symmetry

Increasing # Elastic const.

# Reduction of Elastic Constants with Increasing Symmetry

- A clear explanation of the reduction in the number of elastic constants due to crystal symmetry is provided in Chapter 6 of Wagoner and Chenot (pp. 196-207).
- Excellent explanations are also provided in Nye (i.e., Ch. 8 and Appendix B) and in Reid (Ch. 3).
- You are urged, but not required, to review some of this material.

# Form of the elastic constant matrices for different symmetries

Normal stress X Shear Strain
Shear Stress in a plane X
Shear in another plane

- • Zero component ($s = 0$, $c = 0$)
- ● Non-zero component ($s \neq 0$, $c \neq 0$)
- ●—● Equal components
- ●—○ Numerically equal but opposite
- ●—⊙ ⊙ = 2● for $s$; ⊙ = ●/2 for $c$
- ✖ ✖=$2(s_{11} - s_{22})$ or $(c_{11} - c_{22})/2$

*Figure adapted from J.F. Nye, Physical Properties of Crystals, Oxford University Press (1985), p. 140-141.*

# Cubic Symmetry and Elastic Constants

- Application of a stress along the [100] direction evokes a certain elastic response. Stresses applied along the [010] or [001] axes will evoke an equivalent elastic response. Thus:

  $C_{11} = C_{22} = C_{33}$

- Similarly, applied shear stresses will evoke equivalent responses along the following axes:

  $C_{44} = C_{55} = C_{66}$; $C_{12} = C_{13} = C_{23}$

- The number of independent elastic constants for a cubic material is 3.

# Isotropy considerations

- Cubic materials are not necessarily isotropic.

- For these systems, anisotropy is defined by the Zener ratio, *A*:

$$A = \boxed{\begin{array}{c} (C_{11} - C_{12})/2C_{44} \\ \text{or} \\ 2(S_{11} - S_{12})/S_{44} \end{array}}$$

NOTE: Some books (Ex., Hertzberg) present an inverted version of this equation. However, the implications are still the same.

- When the Zener ratio = 1, the material is isotropic.

# FOR CUBIC SOLIDS

$$\begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ \cdot & C_{11} & C_{12} & 0 & 0 & 0 \\ \cdot & \cdot & C_{11} & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & C_{44} & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & C_{44} & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & C_{44} \end{pmatrix}$$

$$C_{44} = \frac{C_{11} - C_{22}}{2}$$

$$\begin{pmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ \cdot & S_{11} & S_{12} & 0 & 0 & 0 \\ \cdot & \cdot & S_{11} & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & S_{44} & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & S_{44} & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & S_{44} \end{pmatrix}$$

$$S_{44} = 2(S_{11} - S_{22})$$

We can assume that <u>most</u> polycrystalline solids are isotropic but not all.

# Many parameters are used to describe the elastic properties of materials

$$E = \frac{1}{S_{11}} \qquad G = \frac{1}{S_{44}} = \frac{1}{2\left(S_{11} - S_{12}\right)} \qquad \nu = -\frac{S_{12}}{S_{11}}$$

These expressions are for isotropic solids. They are interrelated

$$G = \frac{E}{2\left(1+\nu\right)}$$

See Ch. 8 in Nye, Ch. 13 in Newnham, or Ch. 10 in Gersten for a more thorough explanation.

Wikipedia also provides a nice discussion.

# Elastic Moduli in Cubic Materials

We can use the different relations among elastic constants to ascertain elastic moduli in any crystallographic orientation

$$\frac{1}{E_{hkl}} = S_{11} - 2\left(S_{11} - S_{12} - \frac{1}{2}S_{44}\right)\left(\alpha^2\beta^2 + \beta^2\gamma^2 + \alpha^2\gamma^2\right)$$

Where $\alpha$, $\beta$, and $\gamma$ are the direction cosines between the $[hkl]$ crystal direction and the [100], [010], and [001] directions (*i.e.*, the $x,y,z$ axes).

$\alpha = \cos(\angle[hkl][100])$ ; $\beta = \cos(\angle[hkl][010])$ ; $\gamma = \cos(\angle[hkl][010])$

**TABLE 1.3 Stiffness and Compliance Constants for Selected Crystals**[a]

| Material | $c_{11}$ ($10^{10}$ Pa) | $c_{12}$ | $c_{44}$ | $s_{11}$ ($10^{-11}$ Pa$^{-1}$) | $s_{12}$ | $s_{44}$ |
|---|---|---|---|---|---|---|
| *Cubic* | | | | | | |
| Aluminum | 10.82 | 6.13 | 2.85 | 1.57 | −0.57 | 3.51 |
| Copper | 16.84 | 12.14 | 7.54 | 1.50 | −0.63 | 1.33 |
| Gold | 18.60 | 15.70 | 4.20 | 2.33 | −1.07 | 2.38 |
| Iron | 23.70 | 14.10 | 11.60 | 0.80 | −0.28 | 0.86 |
| Lithium fluoride | 11.2 | 4.56 | 6.32 | 1.16 | −0.34 | 1.58 |
| Magnesium oxide | 29.3 | 9.2 | 15.5 | 0.401 | −0.096 | 0.648 |
| Molybdenum[b] | 46.0 | 17.6 | 11.0 | 0.28 | −0.08 | 0.91 |
| Nickel | 24.65 | 14.73 | 12.47 | 0.73 | −0.27 | 0.80 |
| Sodium chloride[b] | 4.87 | 1.26 | 1.27 | 2.29 | −0.47 | 7.85 |
| Spinel ($MgAl_2O_4$) | 27.9 | 15.3 | 15.3 | 0.585 | −0.208 | 0.654 |
| Titanium carbide[b] | 51.3 | 10.6 | 17.8 | 0.21 | −0.036 | 0.561 |
| Tungsten | 50.1 | 19.8 | 15.14 | 0.26 | −0.07 | 0.66 |
| Zinc sulfide | 10.79 | 7.22 | 4.12 | 2.0 | −0.802 | 2.43 |

| | $c_{11}$ | $c_{12}$ | $c_{13}$ | $c_{33}$ | $c_{44}$ | $s_{11}$ | $s_{12}$ | $s_{13}$ | $s_{33}$ | $s_{44}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| *Hexagonal* | | | | | | | | | | |
| Cadmium | 12.10 | 4.81 | 4.42 | 5.13 | 1.85 | 1.23 | −0.15 | −0.93 | 3.55 | 5.40 |
| Cobalt | 30.70 | 16.50 | 10.30 | 35.81 | 7.53 | 0.47 | −0.23 | −0.07 | 0.32 | 1.32 |
| Magnesium | 5.97 | 2.62 | 2.17 | 6.17 | 1.64 | 2.20 | −0.79 | −0.50 | 1.97 | 6.10 |
| Titanium | 16.0 | 9.0 | 6.6 | 18.1 | 4.65 | 0.97 | −0.47 | −0.18 | 0.69 | 2.15 |
| Zinc | 16.10 | 3.42 | 5.01 | 6.10 | 3.83 | 0.84 | 0.05 | −0.73 | 2.84 | 2.61 |

[a] Data adapted from H. B. Huntington, *Solid State Physics*, Vol. 7, Academic, New York, 1958, p. 213, and K. H. Hellwege, *Elastic, Piezoelectric and Related Constants of Crystals*, Springer-Verlag, Berlin, 1969, p. 3.

[b] Note that $E_{100} > E_{111}$.

R.W. Hertzberg, Deformation & Fracture Mechanics of Engineering Materials, 4th ed., (John Wiley & Sons, New York, 1996) p. 14.

# Elastic properties of polycrystals

- In single crystals elastic constants are determined by bonding between atoms. As such, most single crystals are mechanically anisotropic.

- In polycrystals, the anisotropic behavior of each grain "averages out" because: (a) grain orientations tend to be random; and (b) the deformation of one grain is dependent on the deformation of its neighbor.

- Exceptions occur when the material is textured (i.e., the grains exhibit a preferred orientation).

- Page 34 in Hosford lists some possibilities.

# Elastic Waves in Cubic Crystals

Equation of Motion in X direction

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial X_x}{\partial x} + \frac{\partial X_y}{\partial y} + \frac{\partial X_z}{\partial z}$$

$$\rho \frac{\partial^2 u}{\partial t^2} = C_{11} \frac{\partial e_{xx}}{\partial x} + C_{12} \left( \frac{\partial e_{yy}}{\partial x} + \frac{\partial e_{zz}}{\partial x} \right) + C_{44} \left( \frac{\partial e_{xy}}{\partial y} + \frac{\partial e_{zx}}{\partial z} \right)$$

Equations of Motion

$$\rho \frac{\partial^2 u}{\partial t^2} = C_{11} \frac{\partial^2 u}{\partial x^2} + C_{44} \left( \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + (C_{12} + C_{44}) \left( \frac{\partial^2 v}{\partial x\, \partial y} + \frac{\partial^2 w}{\partial x\, \partial z} \right)$$

$$\rho \frac{\partial^2 v}{\partial t^2} = C_{11} \frac{\partial^2 v}{\partial y^2} + C_{44} \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial z^2} \right) + (C_{12} + C_{44}) \left( \frac{\partial^2 u}{\partial x\, \partial y} + \frac{\partial^2 w}{\partial y\, \partial z} \right)$$

$$\rho \frac{\partial^2 w}{\partial t^2} = C_{11} \frac{\partial^2 w}{\partial z^2} + C_{44} \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right) + (C_{12} + C_{44}) \left( \frac{\partial^2 u}{\partial x\, \partial z} + \frac{\partial^2 v}{\partial y\, \partial z} \right)$$

# Elastic Waves in Cubic Crystals

Waves in the [100] Direction

One solution is given by a longitudinal wave $u = u_0 \exp\left[i(Kx - \omega t)\right]$

$$\omega^2 \rho = C_{11} K^2$$

the velocity /K of a longitudinal wave in the [100] direction is

$$v_s = \nu\lambda = \omega/K = (C_{11}/\rho)^{1/2}$$

Wave in [100] direction
$L : C_{11}$
$T : C_{44}$

Wave in [110] direction
$L : \frac{1}{2}(C_{11} + C_{12} + 2C_{44})$
$T_1 : C_{44}$
$T_2 : \frac{1}{2}(C_{11} - C_{12})$

Wave in [111] direction
$L : \frac{1}{3}(C_{11} + 2C_{12} + 4C_{44})$
$T : \frac{1}{3}(C_{11} - C_{12} + C_{44})$

# Temperature dependence of elastic moduli

- Young's modulus does vary with temperature.

- For metals and ceramics there are some general rules of thumb for temperatures lower than half of the melting temperature.

$$\text{Metals:}\quad E(T) = E(0\ \text{K}) \cdot \left(1 - 0.5\frac{T}{T_{mp}}\right)$$

$$\text{Ceramics:}\quad E(T) = E(0\ \text{K}) \cdot \left(1 - 0.3\frac{T}{T_{mp}}\right)$$

- Different rules apply for polymers.

# Origin of T dependence

- Raising *T* increases the energy of the atoms by an amount $U_t$ causing them to oscillate about their equilibrium positions.
- The repulsive interaction is short range in comparison to the attractive interaction.
- The mean distance between atoms thus grows when temperature is increased due to oscillation.
- Thermal expansion increases and *E* decreases with increasing *T*.

**Young's modulus also tends to scale with $T_{mp}$ for similar reasons.**

# Influence of alloying

- Alloying generally has little influence on the stiffness of materials. This is because the solubility of alloying elements is generally very small (<10%).

- As noted by Roesler et al., the elastic modulus for Al alloys varies by roughly 10% while their strengths can be significantly altered by alloying.

- The Cu-Ni system is an exception to the rule. Ni is 100% soluble in Ni.

[Roesler, p. 41]

# 材料的弹性性质模拟

**Stress-Strain Curve**

Stress tensor

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix}$$

Strain tensor

$$\begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{xy} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{xz} & \epsilon_{yz} & \epsilon_{zz} \end{bmatrix}$$

Stress-Strain relation

$$\sigma_{\mathrm{ij}} = \sum \mathrm{C}_{\mathrm{ijk}l}\, \varepsilon_{\mathrm{kl}}$$

Elastic constant

Unstrained Deformed

$$\mathbf{x}' = (1+\epsilon_{xx})\hat{\mathbf{x}} + \epsilon_{xy}\hat{\mathbf{y}} + \epsilon_{xz}\hat{\mathbf{z}} \;\; ;$$
$$\mathbf{y}' = \epsilon_{yx}\hat{\mathbf{x}} + \left(1+\epsilon_{yy}\right)\hat{\mathbf{y}} + \epsilon_{yz}\hat{\mathbf{z}} \;\; ;$$
$$\mathbf{z}' = \epsilon_{zx}\hat{\mathbf{x}} + \epsilon_{zy}\hat{\mathbf{y}} + (1+\epsilon_{zz})\hat{\mathbf{z}} \;\; .$$

$\epsilon_{\alpha\beta}$ define the deformation; they are dimensionless and have values << 1 if the strain is small

# 模拟流程

**确定平衡结构**

**0 K　Lattice Relaxation**

**Finite Temperature NPT MD**

**计算Stress Tensor**

**基于经验势计算**

**构建 Strain Stress relation**

01

02

03

04

05

06

**微扰晶胞**

**通常是3个Normal、**
**3个 Shear**

**确定Strain tensor**

**注意Strain tensor 三个**
**Shear 分量**

**重复02-05**
**求解弹性常数**

**最少需要六次**

# 1. 确定平衡结构

0 K - 晶胞优化

有限温度- NPT 分子动力学

# 2. 微扰晶胞

定义一个 deformation gradient 矩阵$F$，

$$F = \begin{bmatrix} F_{xx} & F_{yx} & F_{zx} \\ F_{xy} & F_{yy} & F_{zy} \\ F_{xz} & F_{yz} & F_{zz} \end{bmatrix} = \begin{bmatrix} 1 & \delta & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

将$F$与原始晶胞相乘得到deform以后的新晶胞，

$$\begin{bmatrix} a_{2x} & b_{2x} & c_{2x} \\ a_{2y} & b_{2y} & c_{2y} \\ a_{2z} & b_{2z} & c_{2z} \end{bmatrix} = \begin{bmatrix} F_{xx} & F_{yx} & F_{zx} \\ F_{xy} & F_{yy} & F_{zy} \\ F_{xz} & F_{yz} & F_{zz} \end{bmatrix} \begin{bmatrix} a_{1x} & b_{1x} & c_{1x} \\ a_{1y} & b_{1y} & c_{1y} \\ a_{1z} & b_{1z} & c_{1z} \end{bmatrix}$$

以fcc为例，

$$\begin{bmatrix} a & a\delta & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{bmatrix} = \begin{bmatrix} 1 & \delta & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{bmatrix}$$

**注意：　微扰完晶胞需要对原子位置进行优化**

**0K　结构优化**
**有限温度　NVT 分子动力学**

# 3. 计算 Stress Tensor

对晶格施加微小应变，计算应变后的总能量 $E(\epsilon)$

计算 Stress Tensor：

- Numerical : Finite difference

计算量较大，因为需要对系统进行多次微小扰动，每次扰动都需要重新计 算能量或力，因此计算速度较慢，且数值精度受限于微小扰动的大小。

- Analytical : Depends on the energy functional

在有限温度下，材料的能量$E$对体积$V$和晶格变形参数的导数可以得到应力张量的表达式。考虑到体积变形和剪切变形，应力张量的表达为：

$$\sigma_{\alpha\beta} = \frac{1}{V}\frac{\partial E}{\partial \epsilon_{\alpha\beta}}$$

其中， $\epsilon_{\alpha\beta}$是应变张量的分量

# 4. 确定 Strain Tensor

**小应变理论**中的应变定义在连续介质力学中可以用变形梯度张量$F$表示：

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) = \frac{1}{2}\left(F_{ij} + F_{ji}\right) - \delta_{ij}$$

只关注形变影响，通过Green-Lagrange strain tensor的推导，我们可以得到，

$$E = \frac{1}{2}\left(F^T F - I\right)$$

放到小应变假设下，就可以省去二阶以上的高阶项，就有$E \approx \varepsilon$

从而可以得到Strain Tensor的各个分量，继而得到Stress Tensor

# 5. Stress - Strain relation

Stiffness张量通过弹性常数$C_{ij}$将Stress分量与Strain分量关联起来

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

Strain分量 "ε" 和Stress分量 "σ" 由上述表达式通过一组方程联系起来,这些方程中的未知数是弹性常数$C_{ij}$。在下一步中,我们将收集更多这样的方程,直到我们拥有足够多的方程组来找到所有的$C_{ij}$。

# 6. 求解弹性常数

使用彼此独立的deformation，直到完成6种deformation。任何6种deformation的组合都是可以的，只要它们是独立的

$$F_1 = \begin{bmatrix} 1+\delta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad F_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1+\delta & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad F_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1+\delta \end{bmatrix}$$

$$F_4 = \begin{bmatrix} 1 & \delta & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad F_5 = \begin{bmatrix} 1 & 0 & \delta \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad F_6 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \delta \\ 0 & 0 & 1 \end{bmatrix}$$

$F_1$ - $F_3$ 代表 tensile deformations， $F_4$ - $F_6$ 代表 shear deformation.

# 6. 求解弹性常数

为这6种deformation各自写出Stress-Strain relation，并将它们以矩阵形式表示。

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} & \sigma_{15} & \sigma_{16} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} & \sigma_{24} & \sigma_{25} & \sigma_{26} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} & \sigma_{34} & \sigma_{35} & \sigma_{36} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_{44} & \sigma_{45} & \sigma_{46} \\ \sigma_{51} & \sigma_{52} & \sigma_{53} & \sigma_{54} & \sigma_{55} & \sigma_{56} \\ \sigma_{61} & \sigma_{62} & \sigma_{63} & \sigma_{64} & \sigma_{65} & \sigma_{66} \end{bmatrix}$$

在这个方程中要特别注意指标。在stress tensor 和 strain tensor $\sigma_{\mathrm{ij}}$ 或 $\varepsilon_{\mathrm{ij}}$ 中，这里ij作为index的含义，与我们至之前使用的ij含义不同。列指标 j 指的是Deformation的编号（第一次Deformation，第二次Deformation,...），而行指标 i 指的是在Voigt表示法中的位置，如$\sigma_{24}$是第四次变形的$\sigma_{yy}$分量。

$$= \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} & \epsilon_{14} & \epsilon_{15} & \epsilon_{16} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} & \epsilon_{24} & \epsilon_{25} & \epsilon_{26} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} & \epsilon_{34} & \epsilon_{35} & \epsilon_{36} \\ \epsilon_{41} & 2\epsilon_{42} & 2\epsilon_{43} & 2\epsilon_{44} & 2\epsilon_{45} & 2\epsilon_{46} \\ 2\epsilon_{51} & 2\epsilon_{52} & 2\epsilon_{53} & 2\epsilon_{54} & 2\epsilon_{55} & 2\epsilon_{56} \\ 2\epsilon_{61} & 2\epsilon_{62} & 2\epsilon_{63} & 2\epsilon_{64} & 2\epsilon_{65} & 2\epsilon_{66} \end{bmatrix}$$

# 6. 求解弹性常数

如果使用之前推荐的Deformation模式.则我们得到上式右边的矩阵$E$,

$$E = \begin{bmatrix} \delta_1 + \frac{\delta_1^2}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \delta_1 + \frac{\delta_1^2}{2} & 0 & \frac{\delta_2^2}{2} & 0 & 0 \\ 0 & 0 & \delta_1 + \frac{\delta_1^2}{2} & 0 & \frac{\delta_2^2}{2} & \frac{\delta_2^2}{2} \\ 0 & 0 & 0 & 0 & 0 & \delta_2 \\ 0 & 0 & 0 & 0 & \delta_2 & 0 \\ 0 & 0 & 0 & \delta_2 & 0 & 0 \end{bmatrix}$$

这时我们只需要求解矩阵$E$的逆。在上式左右两边同时乘以$E^{-1}$，我们就可以得到Stiffness tensor:

$$\Sigma E^{-1} = C$$

课程作业

1. 推导为什么弹性常数只有21个独立矩阵元