PHYSICS OF MATERIALS

Physics School Autumn 2024

Solutions to Exercise Series 8 **22 November 2024**

Exercise 1 Interaction force between two Shockley partial dislocations

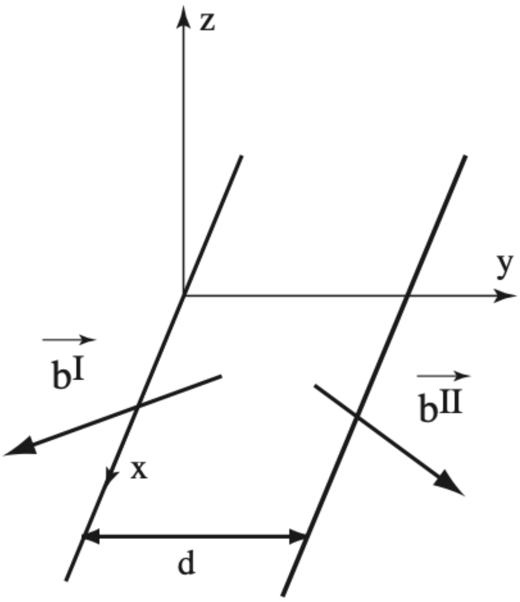

Fig 8.1 Coordinate scheme

Figure 8.1 indicates how to set the dislocations in the coordinate system. We use the Peach and Koehler formula to obtain the force exerted on dislocation II by dislocation I.

$$\vec{F}_{I-II} = \overrightarrow{b^{II}} \cdot \overline{\overline{\sigma^{I}}} \wedge \overrightarrow{t^{II}}$$

The two Burgers vectors $\overrightarrow{b^{I}}$ and $\overrightarrow{b^{II}}$ have a component parallel (screw) to the respective lines of the two partial dislocations and a perpendicular component (edge).

$$\overrightarrow{b^{I}} = \begin{pmatrix} b_s^{I} & b_e^{I} & 0 \end{pmatrix} \qquad \overrightarrow{b^{II}} = \begin{pmatrix} b_s^{II} & b_e^{II} & 0 \end{pmatrix}$$

The stress tensor of the dislocation I having as main axis *x* is (equation 7.13):

$$\sigma^{I} = \sigma^{Is} + \sigma^{Ie} = \begin{pmatrix} 0 & \sigma_{xy}^{s} & \sigma_{xz}^{s} \\ \sigma_{xy}^{s} & 0 & 0 \\ \sigma_{xz}^{s} & 0 & 0 \end{pmatrix} + \begin{pmatrix} \sigma_{xx}^{e} & 0 & 0 \\ 0 & \sigma_{yy}^{e} & \sigma_{yz}^{e} \\ 0 & \sigma_{yz}^{e} & \sigma_{zz}^{e} \end{pmatrix} = \begin{pmatrix} \sigma_{xx}^{e} & \sigma_{xy}^{s} & \sigma_{xz}^{s} \\ \sigma_{xy}^{s} & \sigma_{yy}^{e} & \sigma_{yz}^{e} \\ \sigma_{xz}^{s} & \sigma_{yz}^{e} & \sigma_{zz}^{e} \end{pmatrix}$$

$$\overrightarrow{b^{II}} \cdot \overline{\overline{\sigma^{I}}} = \begin{pmatrix} b_s^{II}\sigma_{xx}^{e} + b_e^{II}\sigma_{xy}^{s} \\ b_s^{II}\sigma_{xy}^{s} + b_e^{II}\sigma_{yy}^{e} \\ b_s^{II}\sigma_{xz}^{s} + b_e^{II}\sigma_{yz}^{e} \end{pmatrix}$$

$\overrightarrow{t^{II}} = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$ and we calculate with the cross product:

$$\vec{F}_{I-II} = \begin{pmatrix} 0 \\ f_y \\ f_z \end{pmatrix} = \begin{pmatrix} 0 \\ b_s^{II}\sigma_{xz}^{s} + b_e^{II}\sigma_{yz}^{e} \\ -\left(b_s^{II}\sigma_{xy}^{s} + b_e^{II}\sigma_{yy}^{e}\right) \end{pmatrix}$$

We use the expressions related to the stress field around an infinite screw or edge dislocation (sections§ 7.5 and 7.13 of the course textbook). Be aware of the reference axis system; the formulas are obtained with a circular permutation $z \rightarrow x, x \rightarrow y, y \rightarrow z$.

$$\sigma_{xy}^{s} = -\frac{\mu b^{I}}{2\pi}\frac{z}{z^2+y^2} = 0$$

$$\sigma_{xz}^{s} = \frac{\mu b^{I}}{2\pi}\frac{y}{y^2+z^2} = \frac{\mu b^{I}}{2\pi d}$$

$$\sigma_{yy}^{e} = -D\frac{\sin\theta(2+\cos 2\theta)}{r} = 0$$

since $\theta = 0$. It's the same for σ_{xx}^{e} and σ_{zz}^{e}

$$\sigma_{yz}^{e} = D\frac{\cos\theta\cos 2\theta}{r} = \frac{D}{y} = \frac{\mu b^{I}}{2\pi(1-\nu)}\frac{1}{d}$$

Therefore $\vec{F}_{I-II} = \begin{pmatrix} 0 & f_y & 0 \end{pmatrix}$ and:

$$f_y = b_e^{II}\sigma_{yz}^{e} + b_s^{II}\sigma_{xz}^{s} = \frac{\mu}{2\pi d}\left(\frac{b_e^{I}b_e^{II}}{1-\nu} + b_s^{I}b_s^{II}\right)$$

It's the formula (7.38) of the course textbook.

2) Calculate the Burgers vectors' components of the partial dislocations following a chosen axis system.

We consider a perfect dislocation of type $\overrightarrow{AB} = \frac{a}{2}[\bar{1}10]$ the dislocation line parallel to *x*.

i)If this dislocation is of screw type, $\overrightarrow{AB}$ is parallel to *x*. We choose the *z*-axis parallel to *(111)* and $\vec{y} = \vec{z} \wedge \vec{x} = \frac{1}{\sqrt{6}}[\bar{1}\bar{1}2]$. The decomposition of $\overrightarrow{AB}$ is made in the plane *(111)* perpendicular to *z,* and the calculation of the basis vectors can be verified on your Thompson tetrahedron. The Thompson tetrahedron gives $\overrightarrow{AB} = \overrightarrow{A\delta} + \overrightarrow{\delta B}$.

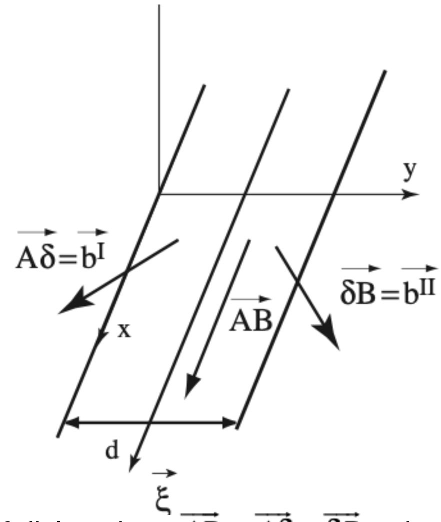

Fig. 8.2 Schematic drawing of dislocations $\overrightarrow{AB} = \overrightarrow{A\delta} + \overrightarrow{\delta B}$ where $\overrightarrow{AB}$ is the screw segment

The Burgers vector of the partial dislocation $\overrightarrow{A\delta} = \frac{a}{6}\left[\bar{1}2\bar{1}\right]$ is calculated according to :

$$b_x = b_s^I = \overrightarrow{A\delta} \cdot \frac{\overrightarrow{AB}}{\left\|\overrightarrow{AB}\right\|} = \frac{a}{2\sqrt{2}} \qquad b_y = b_e^I = \overrightarrow{A\delta} \cdot \frac{\vec{y}}{\left\|\vec{y}\right\|} = \frac{-a}{2\sqrt{6}}$$

The conservation of the Burgers vector allows us to calculate the components of the Burgers vector $\left(b_s^{II}, b_e^{II}\right)$ of $\overrightarrow{\delta B}$:

$$b_s^{II} = b_s^I \quad \text{and} \quad b_e^{II} = -b_e^I$$

$$f_y = \frac{\mu a^2}{2\pi d}\left[-\frac{1}{24}\frac{1}{1-\nu} + \frac{1}{8}\right] = \frac{\mu a^2}{48\pi d}\left[\frac{2-3\nu}{1-\nu}\right]$$

ii) If the dislocation AB is of edge type, the projections of its Burgers vector on the x and y-axis are given by the same calculations.

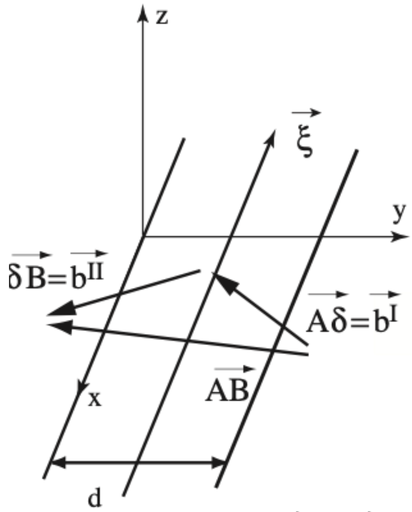

Fig. 8.3 Schematic drawing of dislocations $\overrightarrow{AB} = \overrightarrow{A\delta} + \overrightarrow{\delta B}$ where $\overrightarrow{AB}$ is an edge.

Here, we can take $\frac{\vec{y}}{||\vec{y}||} = \frac{a}{\sqrt{2}}[1\bar{1}0]$ and $\frac{\vec{x}}{||\vec{x}||} = \frac{\vec{y} \wedge \vec{z}}{||\vec{x}||} = \frac{1}{\sqrt{6}}[\bar{1}\bar{1}2]$

$$b_y = b_e^I = \overrightarrow{A\delta} \cdot \frac{\vec{y}}{||\vec{y}||} = -\frac{a}{2\sqrt{2}} \qquad b_x = b_s^I = \overrightarrow{A\delta} \cdot \frac{\vec{x}}{||\vec{x}||} = -\frac{a}{2\sqrt{6}}$$

The conservation of the Burgers vector gives for the other dislocation $\overrightarrow{\delta B}$:

$b_e^{II} = b_e^I$ and $b_s^{II} = -b_s^I$

and finally:

$$f_y = \frac{\mu a^2}{2\pi d}\left[\frac{1}{8}\frac{1}{1-\nu} - \frac{1}{24}\right] = \frac{\mu a^2}{48\pi d}\left[\frac{2+\nu}{1-\nu}\right].$$

The magnitude of the force is more significant than in the previous case.

Note in both drawings that the Thompson tetrahedron dissociation conventions into partials are respected: looking at the perfect dislocation line in the positive direction (vector $\vec{\xi}$), the partial dislocation $\overrightarrow{A\delta}$ is always on the right and $\overrightarrow{\delta B}$ is on the left.

Exercise 2 Precipitation hardening

The decrease in resistivity can be explained by the fact that the matrix becomes increasingly purer when forming precipitates. By Matthiessen's law (resistivity of a solid containing a solute):

$\rho(T) = \rho_0 + \alpha T$, where: $\rho_0 = \rho_0(c)$ and *c* = concentration of the solid solution (decreasing in our case). The maximum hardness can be explained by a change in the mechanism between cutting precipitates and bypass (see course § 8.7.3).

Here, we make a simplified calculation to get the critical radius of the precipitates corresponding to the transition between the two mechanisms.

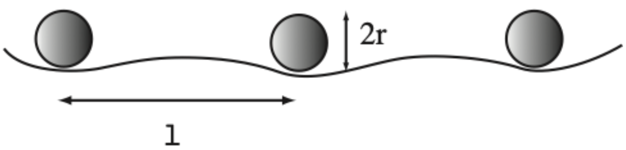

Fig. 8.4 Scheme of a dislocation blocked by precipitates

1) Cutting

The work done by the dislocation to cut the precipitate is given approximately by the force (calculated versus its free length) multiplied by its displacement (2r=d) through the precipitate.

$$\Delta W = \sigma b \ell \cdot 2r$$

This work must equal the needed energy for creating a new interface in the precipitate having an assumed spherical shape, and a circular area (new, created interface) cut the mid-plane of the precipitate. Therefore, we only consider the new interface inside the precipitate, not the matrix precipitate.

$$\Delta E_i = \pi r^2 \gamma_p$$

Therefore $\sigma_{cut} = \dfrac{\pi r \gamma_p}{2b\ell}$

b) Bypass

We can use formula (8.8):

$$\sigma_{byp} = \frac{2\tau}{b\ell} \quad \text{with } \tau \approx 0.5\mu b^2 = \textit{line tension}$$

$$\sigma_{byp} = \frac{\mu b}{\ell}$$

Compared to the example presented in the course textbook and lecture slides, the calculation here of the σ_{byp} doesn't depend explicitly on *r*.

At the maximum hardness $\sigma_{byp} = \sigma_{cut}$:

$$\frac{\pi r_c \gamma_p}{2b\ell} = \frac{\mu b}{\ell}$$

$$r_c = \frac{2\mu b^2}{\pi \gamma_p}$$

The resistivity depends on the number of solute atoms. When all solute atoms have agglomerated and precipitated, the resistivity becomes constant. The hardness continues to decrease since we can have a coalescence process. In reducing the interface energy, the system tends to diminish the total surface of the formed precipitates. If diffusion rates are sufficiently high, small precipitates re-dissolve and precipitate larger particles (e.g., Oswald ripening processes). With this process, the average distance between the precipitates increases.

Since $\sigma_{byp} \propto \dfrac{1}{\ell}$, the hardness decreases. In the case where the precipitates remain small compared to their distance, we then instead use the formula (8.7):

$$\sigma_{byp} = \frac{\tau}{br} \approx \frac{1}{2}\frac{\mu b}{r}$$

In that case, the critical radius slowly grows as a function of the distance between precipitates ℓ since:

$$r_c = b\sqrt{\frac{2\mu\ell}{\pi\gamma_p}}$$

This is the formula (7.38) given in the course text.

Exercise 3 Reaction between dislocations

Vectors $\frac{a}{2}[110]$ and $\frac{a}{2}[1\bar{1}0]$ are perpendicular. Using general assumptions of the theory, we can suppose that the reaction is obtained when the two dislocations are one pure screw and the other pure edge. The energy involved in the reaction is (see § 7.3.1-3 of the course textbook):

$$E\left(\frac{a}{2}[110]+\frac{a}{2}[1\bar{1}0]\right)=\frac{a^2}{2}\ \frac{\mu}{4\pi}\ \ln\ \frac{R}{r_o}+\frac{a^2}{2}\ \frac{\mu}{4\pi(1-\nu)}\ \ln\ \frac{R}{r_o}=$$

$$=\frac{a^2}{2}\frac{\mu}{4\pi}\left(1+\frac{1}{1-\nu}\right)\ln\frac{R}{r_o}=$$

$$\underline{\underline{=\frac{2-\nu}{1-\nu}\frac{a^2}{2}\frac{\mu}{4\pi}\ \ln\ \frac{R}{r_o}}} \qquad (8.3.1)$$

a) The dislocation of Burgers vector $a[100]$ is pure screw:

$$E(a[100])=a^2\frac{\mu}{4\pi}\ln\frac{R}{r_o} \qquad (8.3.2)$$

Thus, considering (8.3.1) and (8.3.2): $\frac{2-\nu}{1-\nu}\cdot\frac{1}{2}=\frac{1-\frac{\nu}{2}}{1-\nu}>1$ and therefore:

$$E(a[100])<E\left(\frac{a}{2}[110]+\frac{a}{2}[1\bar{1}0]\right)$$

The reaction is favorable.

b) The dislocation of Burgers vector $a[100]$ is pure edge:

$$E(a[100])=\frac{1}{1-\nu}a^2\frac{\mu}{4\pi}\ln\frac{R}{r_o} \qquad (8.3.3)$$

Thus, considering (8.3.1) and (8.3.3): $\frac{2-\nu}{1-\nu}\cdot\frac{1}{2}=\frac{1-\frac{\nu}{2}}{1-\nu}<\frac{1}{1-\nu}$ and therefore:

$$E(a[100])>E\left(\frac{a}{2}[110]+\frac{a}{2}[1\bar{1}0]\right)$$

These considerations are valid for usual materials in which $\nu > 0$. In very compressible materials ($K \to 0$), the Poisson ratio becomes negative, and we have the opposite result. Nevertheless, a crystalline material (allowing dislocation formation) with a negative Poisson ratio does not exist. Foams are a class of materials that macroscopically show $\nu < 0$.