1.3 Character of dislocations and Burgers vector

1.3.1 dislocation character and sign

the vector **b** in Fig. 1.7 → Burgers vector

a vector expressing the direction and magnitude of slip caused by the movement of a dislocation

Define a vector **t** : a unit vector parallel to the dislocation line

- **b** ⊥ **t** : edge dislocation
- **b** // **t** : screw dislocation
- otherwise : mixed dislocation

Dislocations have a sign. (Fig. 1.9)

A: positive (+**b**)

B: negative (-**b**)

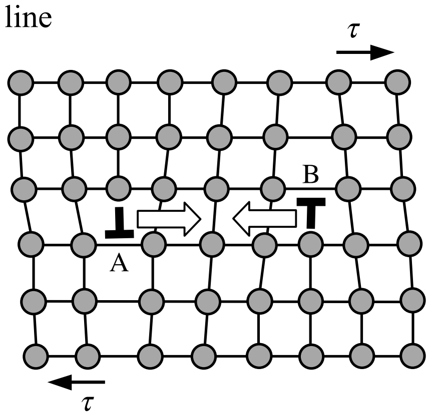

Fig. 1.9 Positive and negative edge dislocations (A and B) move to the opposite directions under applied shear stress τ.

The Burgers vector is an inherent and unique quantity for a given dislocation.

⇓

conservation law of the Burgers vector

1.3.2 Burgers circuit and Burgers vector

Assign **t**.

Assign a starting lattice point S for both crystals with and without a dislocation.

↓

Make a circuit in both crystals so that **t** becomes a proceeding direction of a right-hand screw.

↓

Close the circuit in the crystal with a dislocation so that the finishing point F becomes the same as S.

↓

The same circuit in the perfect crystal results in the creation of a closure failure FS.

↓

The Burgers vector : a vector from F to S.

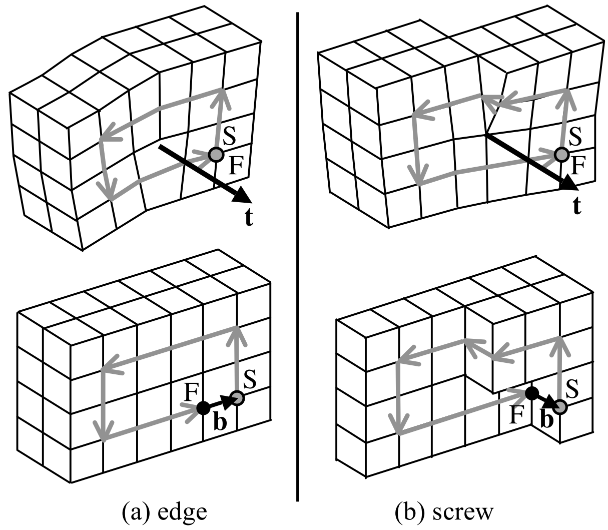

Fig. 1.10 Burgers circuit and Burgers vector

A dislocation never terminate in a crystal. It terminates only at a surface or at a grain boundary.

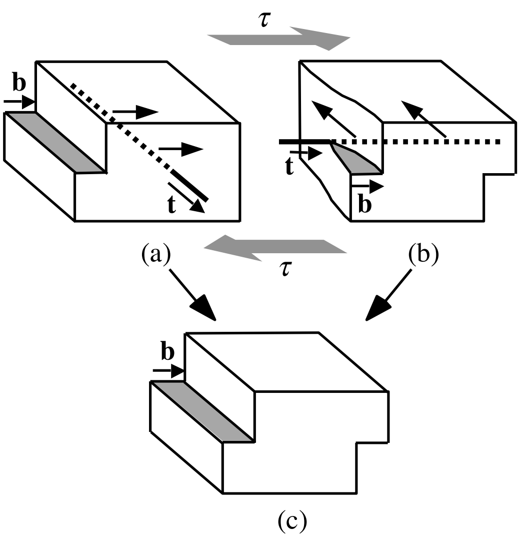

Fig. 1.11 Motion of (a) edge and (b) screw dislocations under applied shear stress τ.

Dislocations are not necessarily straight. They can be curved, branched, etc.

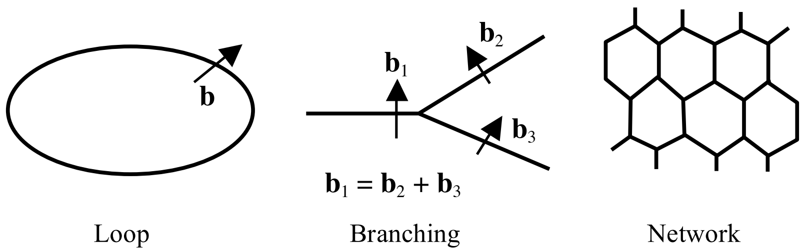

Fig. 1.12 Various dislocation shapes

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Problem 1.4

Smartly and elegantly explain the fact that dislocations never terminate in a crystal.

Problem 1.5

Which dislocation loop is physically possible, an edge dislocation loop or a screw dislocation loop?

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Chapter 2 Elastic Field and Line Tension of a Dislocation

2.1 Elastic field around a dislocation

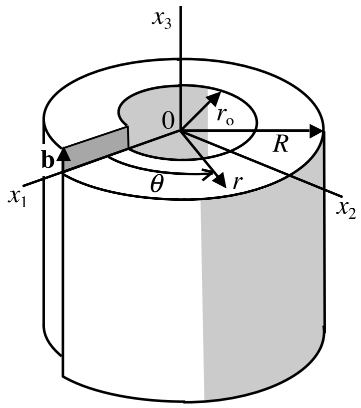

Fig. 2.1 A straight screw dislocation on the x_3 axis.

A straight screw dislocation on the (r, θ, x_3) cylindrical coordinate system.:

The displacement **u** of an arbitrary point $(r, \theta, 0)$ along x_3:

$$u_1 = u_2 = 0$$
$$u_3 = \theta b / (2\pi) = (b / 2\pi) \tan^{-1}(x_2 / x_1) \qquad (2.1)$$

Since the displacement is known, elastic strains e_{ij} can be calculated from $e_{ij} = (u_{i,j} + u_{j,i}) / 2$. Then, from the elastic strains and the Hooke's law, stress components σ_{ij}^{s} can be easily obtained. In the Cartesian coordinate system, they become

$$\sigma_{ij}^{\mathrm{s}} = \begin{bmatrix} 0 & 0 & -\dfrac{\mu b}{2\pi} \dfrac{x_2}{x_1^2 + x_2^2} \\ 0 & 0 & \dfrac{\mu b}{2\pi} \dfrac{x_1}{x_1^2 + x_2^2} \\ -\dfrac{\mu b}{2\pi} \dfrac{x_2}{x_1^2 + x_2^2}, & \dfrac{\mu b}{2\pi} \dfrac{x_1}{x_1^2 + x_2^2}, & 0 \end{bmatrix} \qquad (2.2)$$

where μ is the shear modulus. Or, in the cylindrical system

$$\varepsilon_{\theta x_3} = \varepsilon_{x_3 \theta} = \frac{b}{4\pi r}, \qquad \sigma_{\theta x_3}^{\mathrm{s}} = \sigma_{x_3 \theta}^{\mathrm{s}} = \frac{\mu b}{2\pi r} \qquad (2.3)$$

Elastic field of a dislocation → inversely proportional to the distance from the dislocation The attenuation is rather weak. → long-range stress field

For a straight edge dislocation with t = [0, 0, 1] and **b** = [b, 0, 0]

$$\sigma_{ij}^{\mathrm{e}} = \begin{bmatrix} -\dfrac{\mu b}{2\pi(1-\nu)} \dfrac{x_2(3x_1^2 + x_2^2)}{(x_1^2 + x_2^2)^2} & \dfrac{\mu b}{2\pi(1-\nu)} \dfrac{x_1(x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2} & 0 \\ \dfrac{\mu b}{2\pi(1-\nu)} \dfrac{x_1(x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2} & \dfrac{\mu b}{2\pi(1-\nu)} \dfrac{x_2(x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2} & 0 \\ 0 & 0 & -\dfrac{\mu \nu b}{\pi(1-\nu)} \dfrac{x_2}{x_1^2 + x_2^2} \end{bmatrix} \qquad (2.4)$$

where ν is the Poisson ratio.

2.2 Elastic strain energy of a dislocation

$$E_{\mathrm{el}} = \frac{1}{2}\int_{-\infty}^{\infty}\int_{0}^{2\pi}\int_{0}^{\infty}\left(\varepsilon_{\theta x_3}\sigma^{\mathrm{s}}_{\theta x_3} + \varepsilon_{x_3\theta}\sigma^{\mathrm{s}}_{x_3\theta}\right) r\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}x_3 = \int_{-\infty}^{\infty}\int_{0}^{2\pi}\int_{0}^{\infty}\{\mu b^2/(8\pi^2 r^2)\}\, r\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}x_3$$

per unit length

$$E^{\mathrm{s}}_0 = \int_{0}^{2\pi}\int_{0}^{\infty}\{\mu b^2/(8\pi^2 r^2)\}\, r\,\mathrm{d}r\,\mathrm{d}\theta = \frac{2\pi\mu b^2}{8\pi^2 r^2}\int_0^{\infty}\left(\frac{1}{r}\right)\mathrm{d}r$$

by setting the upper and lower bounds of the integral as r_0 and R

$$E^{\mathrm{s}}_0 = \frac{\mu b^2}{4\pi}\ln\left(\frac{R}{r_0}\right), \quad \text{(screw dislocation)} \tag{2.5}$$

r_0 ($\approx 5b$) : dislocation core radius, R : crystal radius or grain radius

Similarly,

$$E^{\mathrm{e}}_0 = \frac{\mu b^2}{4\pi(1-\nu)}\ln\left(\frac{R}{r_0}\right), \quad \text{(edge dislocation)} \tag{2.6}$$

Very rough expression

$$\boxed{E_0 = \alpha\mu b^2} \; (\alpha \approx 1/2 \text{ to } 1, \text{ regardless of dislocation character}) \tag{2.7}$$

2.3 Line tension

string model of a dislocation with line tension T_{L}

$$\boxed{T_{\mathrm{L}} \approx E_0 \approx \mu b^2/2} \tag{2.8}$$

Problem 2.1

(1) Using $r_{\mathrm{o}} = 10^{-9}\,\mathrm{m}$ and $R = 10^{-6}\,\mathrm{m}$ as well as Eq. (2.5), calculate α in Eq. (2.7) for a screw dislocation.

(2) For Cu ($\mu = 4.6\times10^{10}\,\mathrm{Pa}$, $b = 0.255\,\mathrm{nm}$), what will be the elastic strain energy of the above screw dislocation with length b? Answer in units of [J] and [eV].
