ME 477/677

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Information from various sources, including Mechanical Metallurgy (Dieter) and Introduction to Dislocations (Hull) and Elementary Dislocation Theory (Weertman and Weertman)

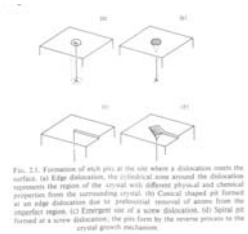
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Observation of Dislocations

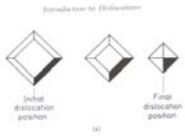
- Dislocations were firs proposed in the 1930s as a mechanism to explain the low yield stress in crystalline materials
- For the following 10 years or so the theory of dislocations was developed without a reliable method of observing them
- Only now are techniques such as HRTEM and AFM becoming sufficiently advanced to be able to resolve individual atoms around dislocations.
- Observation of dislocation is by taking advantage of the distortions or strain fields in the surrounding crystal
  - Chemical methods – etch pits, decoration …
  - Physical methods – TEM, X-Ray …
- Etch pits
  - Impurities tend to segregate to dislocations and are more chemically active (anodic) than the surrounding. When exposed to an acid, pits form where the dislocation intersects the surface
    - Edge dislocation – conical pit
    - Screw dislocation – spiral pit

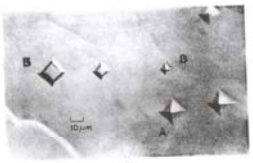
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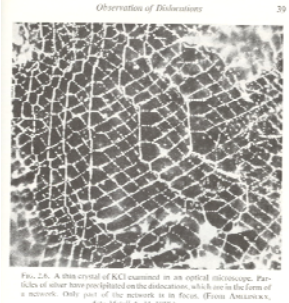




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Observation of Dislocations

- Decoration Techniques
  - In optically transparent crystals, when impurity atoms diffuse to the dislocations and make them visible

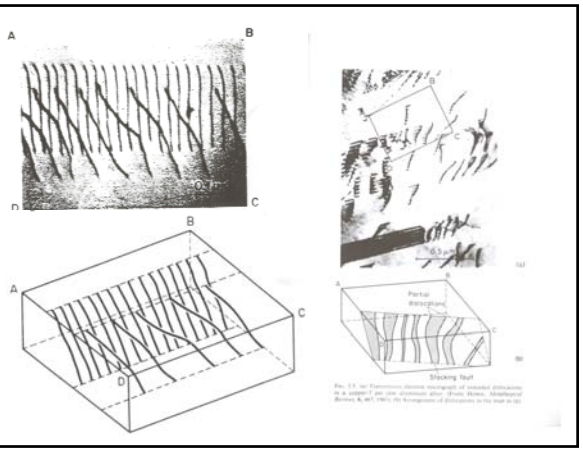


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Observation of Dislocations

- TEM
  - Thin foils ~100 nm thick are transparent to electrons
  - The electron beam interacts with the crystal
  - In the transmitted image, the intensity of the electron beam is altered by the local strain field
  - Dislocations may appear as dark lines (~10 nm wide) in a normally bright area
  - Using kinematic and dynamic theories it is possible to analyze the image to get the line orientation as well as the burgers vector
  - Stacking faults can also be observed

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Dislocation Interactions – Unit and Partial Dislocations

- The burgers vector $\vec{b}$ is a measure of the "strength" of a dislocation
  - the direction and amount of displacement during plastic deformation
- The energy associated with a dislocation is proportional to the square of the burgers vector – this will be shown later
- A unit dislocation is one for which the magnitude of the burgers vector is equal to the distance between adjacent atoms
- Dislocations with burgers vector greater than unity are unstable and will split up into dislocations with smaller burgers vectors
  - A dislocation with a burgers vector of 2b is unstable compared to two dislocations each with a burgers vector of b

$$\left|2\vec{b}\right|^2 = 4b^2 > b^2 + b^2$$

  - Like dislocations repel each other
  - Dislocations with burgers vector < unity are possible. These are called partial dislocations
- A dislocation with burgers vector $\vec{b}_1$ will split into two dislocations with burgers vectors of $\vec{b}_2$ and $\vec{b}_3$ if

$$\vec{b}_1 = \vec{b}_2 + \vec{b}_3$$

and

$$|b_1|^2 > |b_2|^2 + |b_3|^2$$

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Dislocation Interactions – Unit and Partial Dislocation

- For example

$$\frac{a_0}{2}[0\bar{1}1] = \frac{a_0}{6}[1\bar{2}1] + \frac{a_0}{6}[\bar{1}\bar{1}2]$$

$$|b_1|^2 = \left(\frac{a_0}{2}\right)^2\left(1^2 + (-1)^2 + 0^2\right) = \frac{a_0^2}{2}$$

$$|b_2|^2 = \left(\frac{a_0}{6}\right)^2\left(1^2 + (-2)^2 + 1^2\right) = \frac{a_0^2}{6}$$

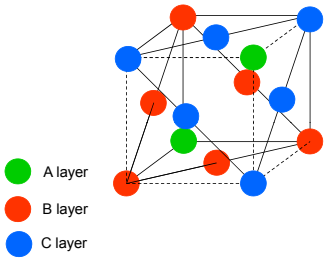
$$|b_3|^2 = \left(\frac{a_0}{6}\right)^2\left((-1)^2 + (-1)^2 + 2^2\right) = \frac{a_0^2}{6}$$

$$|b_2|^2 + |b_3|^2 = \frac{a_0^2}{3} < \frac{a_0^2}{2} = |b_1|^2$$

- The disassociation of the dislocation with burgers vector $\frac{a_0}{2}[0\bar{1}1]$ into two dislocations with burgers vectors $\frac{a_0}{6}[1\bar{2}1]$ and $\frac{a_0}{6}[\bar{1}\bar{1}2]$ is energetically favorable

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Partial Dislocations in FCC



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Partial Dislocations in FCC

$$B_1 = a_0\left(\frac{1}{2}, 0, \frac{1}{2}\right)$$

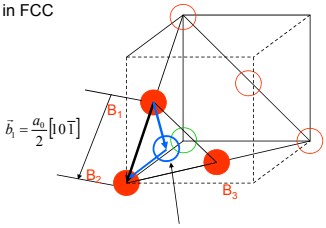
$$B_2 = a_0(1,0,0)$$

$$\vec{b}_1 = B_2 - B_1 = \frac{a_0}{2}[10\bar{1}]$$

$$C = a_0\left(\frac{2}{3}, \frac{1}{6}, \frac{1}{6}\right)$$

$$\vec{b}_2 = B_1C = \frac{a_0}{6}[11\bar{2}]$$

$$\vec{b}_3 = CB_2 = \frac{a_0}{6}[2\bar{1}\bar{1}]$$



C position in the middle of the B triangle

$$\frac{a_0}{2}[10\bar{1}] = \frac{a_0}{6}[11\bar{2}] + \frac{a_0}{6}[2\bar{1}\bar{1}]$$

$$\vec{b}_1 = \vec{b}_2 + \vec{b}_3$$

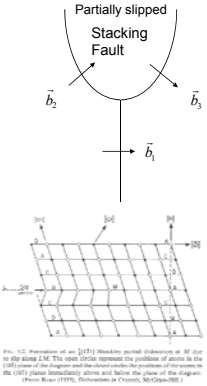
and

$$|b_1|^2 > |b_2|^2 + |b_3|^2$$

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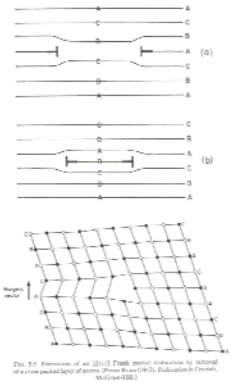
Partial dislocations – Shockley Partials

- The burgers vectors of the two partial dislocations are almost parallel to each other
- The dislocations repel each other and a partially slipped region forms between the two – this is the region of the stacking fault
- These dislocations are called Shockley Partials
- They are mixed dislocations since $\vec{\ell}$ and $\vec{b}$ are neither parallel nor perpendicular to each other
- They are glissile dislocations and will move under an applied stress on the plane of the figure
- Both edge and screw dislocations can split into partials
- When a dislocation splits into partials, it can not change slip planes (by climb or cross slip) since the slip of the partials is confined to the plane of the stacking fault
  - The partials must recombine before cross slip is possible



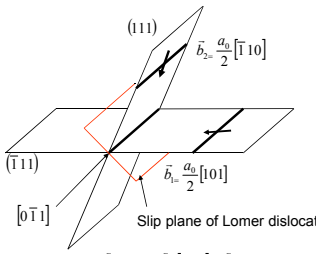
Partial Dislocations – Frank partials

- When a portion of a plane is missing, or a segment of a plane is inserted, the local stacking sequence is disrupted, i.e. a stacking fault is formed
- The ends of the stacking fault are marked by edge dislocations, called Frank partials
- The burgers vectors the dislocations are of the type $\vec{b} = \frac{a_0}{3}[111]$
- The slip plane of these dislocations does not coincide with the plane of the stacking fault.
- Frank partials are sessile
- They can move by climb, i.e. addition or removal of atoms at the end of the "half" planes that bound the stacking fault



Lomer and Lomer-Cottrell Dislocations

- **Lomer Reaction**: When two parallel dislocations gliding on intersecting slip planes encounter each other, they can combine to form a single dislocation with a non-close packed slip plane.

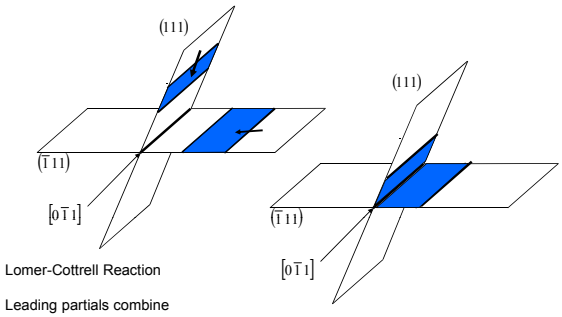


$$\frac{a_0}{2}[101]+\frac{a_0}{2}[\bar{1}10]=\frac{a_0}{2}[011]$$

$$|b_1|^2+|b_2|^2>|b_3|^2$$

Lomer and Lomer-Cottrell Dislocations

- **Lomer-Cottrell Reaction**: If the two dislocations in the Lomer reaction split into partials before they meet, then the leading partials can combine to form a sessile dislocation. The stacking fault is now distributed on two planes, with the Lomer-Cottrell dislocation along the line of intersection of the planes. This is also called a "stair-rod" dislocation analogous to a rod holding a carpet against the steps in a staircase
- Lomer and Lomer-Cottrell barriers can be broken at high temperatures or pressures to recombine the dislocations to eliminate the stacking faults. However the stress required is much higher than that required for cross-slip of screw dislocations



Lomer-Cottrell Reaction

Leading partials combine

$$\frac{a_0}{6}[\bar{1}2\bar{1}]+\frac{a_0}{6}[1\bar{1}2]=\frac{a_0}{6}[011]$$

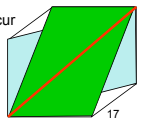
$$|b_1|^2+|b_2|^2>|b_3|^2$$

Dislocation Reactions in other systems

- HCP
  - For (c/a)>1.633, the only slip systems are in the basal plane
  - These dislocations can disassociate the same way as in FCC, resulting in a local region where the ABAB… stacking is disrupted.

$$a[1\bar{1}20]\rightarrow a[10\bar{1}0]+a[01\bar{1}0]$$

- BCC
  - Close packed direction is $\langle 111 \rangle$
  - Burgers vector is $\frac{a_0}{2}\langle 111 \rangle$
  - Three families of planes have the same density of atoms {110}, {112} and {123}
  - Each <111> lies on three {110} – two are shown
  - When {110} slip predominates, then cross slip can occur
  - Deformation of bcc-iron appears wavy

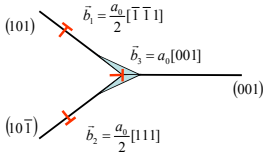


Dislocations in other crystal systems

- BCC
  - One possible dislocation reaction is

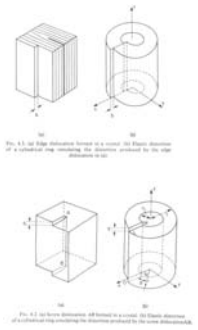
$$\frac{a_0}{2}[\bar{1}\bar{1}1]+\frac{a_0}{2}[111]\rightarrow a_0[001]$$

  - The [001] direction is not close packed and the resultant dislocation is sessile
  - The (001) plane is a cleavage plane – the fracture stress is low
  - These reaction can initiate cracks



Stress Fields and Energies of dislocations

- The presence of a dislocation distorts the crystal
- The interaction between dislocations and other defects, such as dislocations and impurity atoms) depends of the strain and stress fields that develop around a dislocation
- Equations that describe the stress fields around a dislocation can be quite complex due to the anisotropic nature of a crystal unit cell
  - The Volterra model - a highly simplified model assumes the crystal to be an isotropic continuum
  - The region outside the "core" of the dislocation can be modeled as a rubber tube that has been cut and sheared



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Stress Fields and Energies of dislocations

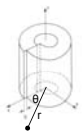
- For an edge dislocation, both shear and normal stresses are present

$$\sigma_r = \sigma_\theta = \frac{-\tau_0 b \sin\theta}{r}$$

$$\tau_{r\theta} = \frac{\tau_0 b \cos\theta}{r}$$

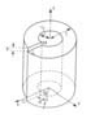
where

$$\tau_0 = \frac{G}{2\pi(1-\nu)}$$



- For a screw dislocation only shear stresses are present

$$\tau_{\theta z} = \frac{Gb}{2\pi r}$$



- These equations are valid only outside the "core" of the dislocation, since stresses go to infinity if *r=0* in the above equations
- The core of a dislocation has a radius

  r_0 = 0.5 to 1 nm or 5 to 10 Å

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Stress Fields and Energies of dislocations

- The strain energy per unit length associated with an edge dislocation can be estimated using Volterra's model as the work done do move a dislocation from the surface of a crystal of radius r_1 to the center.

$$U = \frac{1}{2}\int_{r_0}^{r_1} \tau_{r\theta} b\, dr$$

$$U_{edge} = \frac{G b^2}{4\pi(1-\upsilon)} \ln\frac{r_1}{r_0}$$

$$U_{screw} = \frac{G b^2}{4\pi} \ln\frac{r_1}{r_0}$$

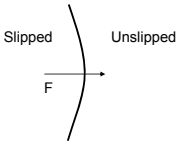
- If there are a number of dislocations present in the crystal, then r_1 = half the average distance between dislocations
- The core of the dislocation has a radius $r_0 \approx b$
- The additional energy present in the core is estimated to be about 0.5eV
- The presence of a dislocation increases the energy in the crystal
  - The crystal is more unstable and annealing removes dislocations

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Forces on Dislocations

- The force acting on a dislocation per unit length when a shear stress of τ is applied is

$$F = \tau . b$$



- Since the energy of a dislocation is proportional to its length, a dislocation can minimize its energy by assuming a straight configuration
  - A curved dislocation will try to straighten itself
  - The stress required to bend a dislocation into an arc of radius R is given by Orowan's equation

$$\tau = \frac{G.b}{2R}$$

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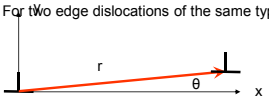
Force between parallel dislocations on parallel slip planes

- The force acting on a dislocation is determined by the product of the burgers vector and the shear stress magnitude
- When two dislocations are on the same plane, the force that they experience depends on the stress field of the other dislocation

$$F_{screw} = \tau_{\theta z} . b = \frac{Gb^2}{2\pi r}$$

$$F_{edge} = \tau_{r\theta} . b = \frac{Gb^2 \cos\theta}{2\pi r(1-\upsilon)}$$

- Like dislocations will repel each other and unlike dislocations will be attracted towards each other
- When there are two dislocations on parallel slip planes, then the resultant force can be attractive or repulsive, depending on their relative position
- For two edge dislocations of the same type

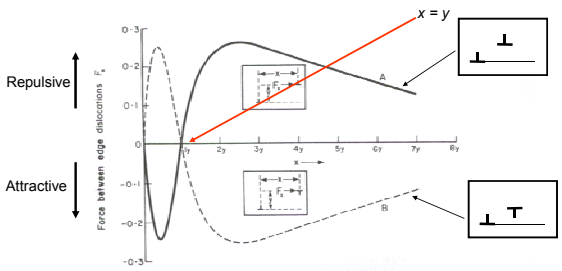


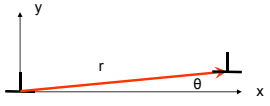
$$F_x = \frac{Gb^2 \cos\theta}{2\pi(1-\upsilon)r} - \frac{Gb^2 \sin 2\theta \sin\theta}{2\pi(1-\upsilon)r}$$

$$= \frac{Gb^2 x\left(x^2 - y^2\right)}{2\pi(1-\upsilon)\left(x^2 + y^2\right)^2}$$

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Force between parallel edge dislocations on parallel slip planes





$$F_x = \frac{Gb_1b_2 \cos\theta}{2\pi(1-\upsilon)r} - \frac{Gb_1b_2 \sin 2\theta \sin\theta}{2\pi(1-\upsilon)r}$$

$$= \frac{\pm Gb^2 x\left(x^2 - y^2\right)}{2\pi(1-\upsilon)\left(x^2 + y^2\right)^2}$$

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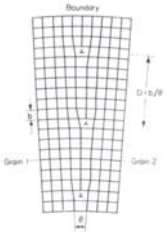
Force between parallel edge dislocations on parallel slip planes

- A positive value of the force indicates repulsion and a negative value attraction
- When the dislocation are far apart, each "sees" the other as being on the same plane and the force is repulsive
- However, when the dislocations approach each other, for θ < 45°, the force becomes attractive
- An arrangement of dislocations lined up one above the other is a minimum energy configuration with no relative force.
  - The strain field of one dislocation is partially neutralized by the strain field of the next
  - This arrangement is called a low angle grain boundary
- The opposite argument applies for unlike dislocations
  - If the dislocations were to line up one above the other, there would have to be a row of vacancies between them

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Low angle grain boundary





Etch pits indicating locations of parallel dislocations stacked one above the other

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Forces between Shockley Partials

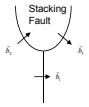
- A pair of Shockley partials with an intervening stacking fault is also called an extended dislocation
- The partial dislocations have almost parallel burgers vectors, and will repel each other extending the width of the stacking fault
- The stacking fault is a crystal defect with an associated energy, and increasing its size will increase the overall energy of the crystal
- If the stacking fault energy per unit area is γ, then the partial dislocations will move apart until
  - The repulsive force per unit length = stacking fault energy/unit area
- Assuming the partial dislocations have only an "edge" character, then

$$F_r = \frac{Gb^2}{2\pi(1-\upsilon)r} = \gamma$$

- Therefore, at equilibrium, the partial dislocations will be at a distance r apart where

$$r = \frac{Gb^2}{2\pi(1-\upsilon)\gamma}$$

- This will also be the width of the stacking fault



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Image Force

- A dislocation that is near a free surface will be attracted to the surface since it can escape the crystal, leaving the crystal defect free
- The attractive force can be calculated by assuming there is a dislocation of opposite sign at the same distance on the other side of the free surface
  - This is called an image dislocation
  - The associated force is called the image force

$$F_{image} = \frac{Gb^2}{4\pi(1-\upsilon)r}$$

- Note: "*r*" is the distance of the dislocation from the free surface. The image dislocation distance is then "2*r*". Therefore the "4" in the denominator

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Dislocation Climb

- Edge dislocations can change their slip plane by "climb"
- "Negative" climb when a row of atoms is added to (or a row of vacancies diffuse away from) the bottom of the half-plane
- "Positive" climb when a row of atoms is removed from (or a row of vacancies diffuse to) the bottom of the half-plane

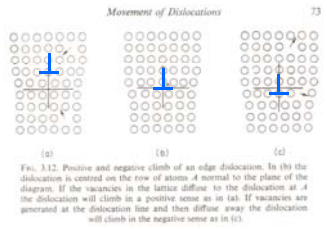


FIG. 3.12. Positive and negative climb of an edge dislocation. In (b) the dislocation is centred on the row of atoms A normal to the plane of the diagram. If the vacancies in the lattice diffuse to the dislocation at A the dislocation will climb in a positive sense as in (a). If vacancies are generated at the dislocation line and then diffuse away the dislocation will climb in the negative sense as in (c).

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Jogs

- Atoms may not be added or removed from the entire length of the dislocation, but only over short segments
  - Jogs are formed along the length of the dislocations
  - The jogs themselves are short edge dislocations that lie entirely within the core of the parent dislocation
- The number of jogs that form along the length of the dislocation is

$$n_j = n_0 \exp\left(\frac{-U_j}{kT}\right)$$

- Where
  - n_j = # of jogs per unit length
  - n_0 = # of atoms per unit length
  - U_j = activation energy to form a jog ~ 1ev
- The activation energy for climb is

$$U_c = U_j + U_v + U_m = U_j + U_d$$

Vacancy creation

Vacancy diffusion

Self diffusion

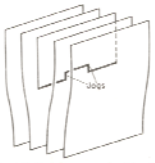


FIG. 3.13. Single jogs on an edge dislocation.

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Jogs

- In a cold worked material, there will be a number of jogs along a dislocation
  - This is discussed later
- The activation energy for climb is therefore controlled by the activation energy for self diffusion

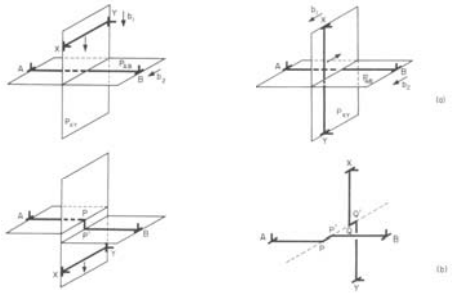
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Intersection of Perpendicular Dislocations

- When perpendicular dislocations intersect, each dislocation gets a step in the direction of the burgers vector of the other
- The step is called a
  - Jog – if the parent dislocation moves out of its original slip plane
  - Kink – if the step keeps the parent dislocation on its original slip plane
- Since jogs and kinks are part of the parent dislocation, they have the same burgers vector as the parent
- Jogs and kinks can be of edge of screw type, depending on the relative orientation of the burgers vector and the jog or kink.

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Intersection of Perpendicular Dislocations – Two Edge dislocations



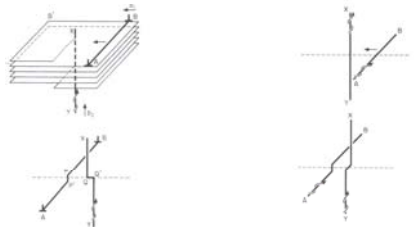
- AB gets an edge-jog
- XY is unaffected

- AB gets a screw-kink
- XY gets a screw-kink

The original shear stresses can cause the stepped dislocations to glide

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Intersection of Perpendicular Dislocations

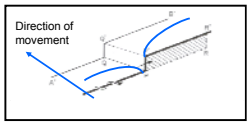


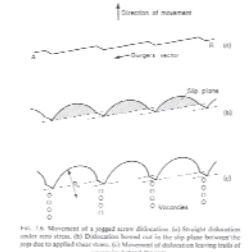
- The edge dislocation gets an edge jog
- The screw dislocation gets an edge kink
- The steps can glide under the same stress as the parent dislocations

- Each dislocation acquires an edge-jog
- The glide planes of the jogs are not the same as those of the screw dislocations

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Movement of a jogged screw dislocation





- Slip plane of PP' is the shaded PP'RR'
- Glide of the screw dislocation will to A'QQ'B' will require PP' to climb to QQ'
- A screw dislocation will acquire many jogs of both, positive and negative
- The jogs will be able to migrate along the length so that jogs of opposite sense will annihilate each other leaving an excess of one type which will be uniformly distributed along the length
- The jogged screw dislocation will move by the screw segments bowing between the jogs and the jogs climbing by leaving a trail of vacancies

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Movement of a jogged screw dislocation

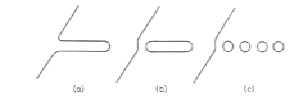


FIG. 7.11. Formation of dislocation loops from a dislocation dipole. (a) Dislocation dipole. (b) Elongated loop and jogged dislocation. (c) Row of small loops.

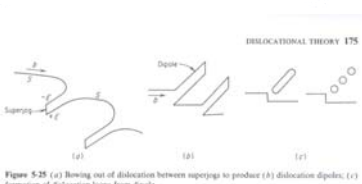
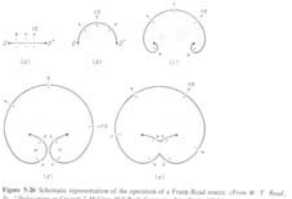


Figure 5-25 (a) Bowing out of dislocation between superjogs to produce (b) dislocation dipoles; (c) formation of dislocation loops from dipole.

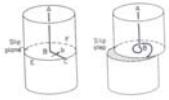
- Formation of
  - Elongated loops
  - Row of small loops
  - Dislocation dipoles
  - Bowing out between super-jogs

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Dislocation Multiplication







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Dislocation-Point Defect Interaction

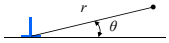
- A point defect, such as a substitutional atom, has a spherically symmetric strain field
  - An atom of size *a'* replaces an atom of size *a*

$$\text{Linear strain } \varepsilon = \frac{(a'-a)}{a}$$

$$\text{Volume strain } \varepsilon_V = 3\varepsilon$$

$$\text{Volume change } \Delta V = \frac{4\pi a^3}{3}\varepsilon_V = 4\pi a^3 \varepsilon$$

- The strain field of the point defect interacts with the stress field of the dislocation
- A spherically symmetric strain field interacts with the hydrostatic component of the stress field
- Consider a point defect at a location (r,θ) from an edge dislocation



- The hydrostatic or mean normal stress is

$$\sigma_m = \frac{(1+\upsilon)Gb\sin\theta}{3\pi(1-\upsilon)r}$$

- Interaction energy is

$$U_i = \sigma_m \Delta V$$

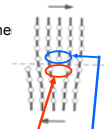
$$U_i = \frac{4(1+\upsilon)Gba^3\varepsilon\sin\theta}{3(1-\upsilon)r} = A\varepsilon\frac{\sin\theta}{r}$$

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Dislocation-Point Defect Interaction

- $U_i > 0 \Rightarrow$ Dislocation and solute atom repel each other
- $U_i < 0 \Rightarrow$ Dislocation and solute atom attracted towards each other

$$U_i = A\varepsilon\frac{\sin\theta}{r}$$



- When ε > 0 (substitutional atom is larger than matrix atom)
  - $U_i > 0$ when $\sin\theta > 0$ i.e. $0 < \theta < \pi$ or above the slip plane - repulsion
  - $U_i < 0$ when $\sin\theta > 0$ i.e. $\pi < \theta < 2\pi$ or below the slip plane - attraction
- When ε < 0 (substitutional atom is smaller than matrix atom)
  - $U_i > 0$ when $\sin\theta < 0$ i.e. $0 < \theta < \pi$ or above the slip plane - attraction
  - $U_i < 0$ when $\sin\theta > 0$ i.e. $\pi < \theta < 2\pi$ or below the slip plane – repulsion
- Large atoms will collect under the bottom of the extra half plane (region of tension)
- Small atoms will collect above the bottom of the extra half plane (region of compr.)



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Dislocation-Point Defect Interaction

- Since a screw dislocation has only a shear stress, it will not interact with the spherically symmetric strain field of a point defect such as a substitutional atom
- Some point defects, such as C in bcc-Fe, have a non-symmetric distortion field. Interactions will occur in this case.

- The concentration of impurities near a dislocation will be higher (or lower) than average when $U_i < 0$ (or $U_i > 0$)
- There is an "impurity cloud" around a dislocation
- In iron, if the carbon atom concentration is high enough that all interstitial sites near dislocations are filled with solute atoms, then the solute atoms are said to have "condensed" on the dislocation lines

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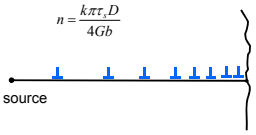
Dislocation Pile-Ups

- Dislocations can be stopped by obstacles, such as grain boundaries, impurity particles, and interaction with other dislocations
- If the dislocations are emanating from a source, then there can be a pile up of dislocations against the barrier
- The result is a back stress on additional dislocations
  - We saw this as the Bauschinger effect earlier
- Under a stress τ, the number of dislocations that can occupy a slip plane of length L between the source and the barrier is

$$n = \frac{k\pi\tau_s L}{Gb}$$

- Where k = 1 for a screw dislocation and k= (1-ν) for an edge dislocation
- If the source is located at the center of a grain of diameter D, then D = 2L
- Since the source feels the back stress from both sides, the above equation becomes

$$n = \frac{k\pi\tau_s D}{4Gb}$$



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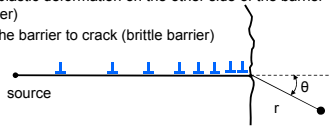
Dislocation Pile-Ups

- The dislocation pile up can be considered to be a single dislocation of strength nb at a distance $3L/4$ from the source
- Large stresses can develop on the other side of the barrier
- The maximum stress occurs for $\theta = 70.5^o$ when

$$\sigma_{max} = \frac{2}{\sqrt{3}}\left(\frac{L}{r}\right)^{(1/2)}\tau_s$$

$$\tau = \beta\tau_s\left(\frac{L}{r}\right)^{(1/2)}$$

- If the stresses get high enough
  - Dislocations may be able to cross-slip or climb around barrier
  - May initiate plastic deformation on the other side of the barrier (ductile barrier)
  - May cause the barrier to crack (brittle barrier)



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