Multiscale Simulations of Materials and Structures

Lecture 7.
Dislocation Dynamics

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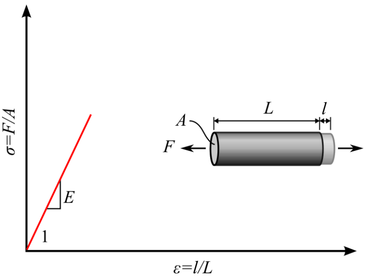
Outline

Introduction

Notion of plasticity

- Plasticity. . . irreversible change of shape
- In metals plasticity is the result of motion of linear defects of the crystal lattice: **dislocations**
- In rocks, for example, the plasticity is caused by slip at microcracks



Adapted from Wikipedia

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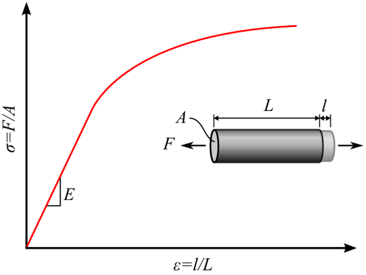

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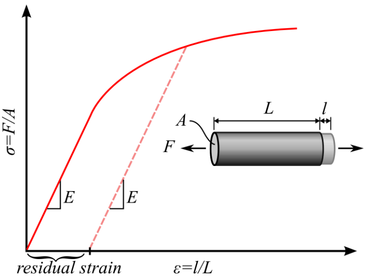

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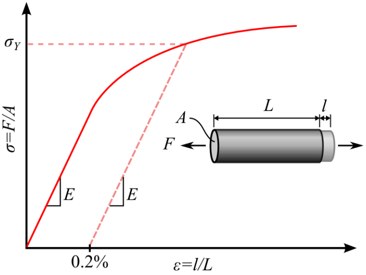

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Notion of plasticity

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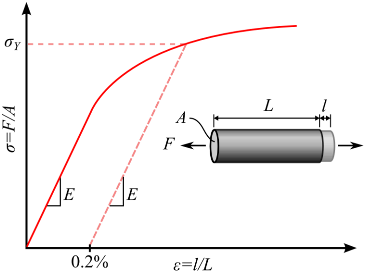
Objective:

- Understand basics of dislocation motion (✓ *for DMS students*)
- Convert this understanding into a computational model: **Dislocation Dynamics**



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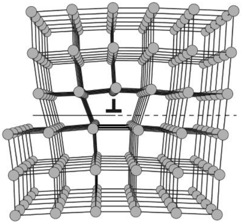
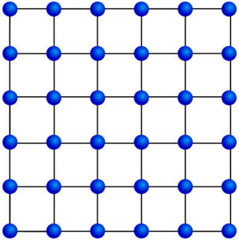


from
[1] Bulatov V.V., Cai W. Computer Simulations of Dislocations, Oxford University Press, 2006.

Basic concept

- Dislocation is a line defect, a curve in a volume
- But the basics can be understood in 2D...



Square lattice

Basic concept

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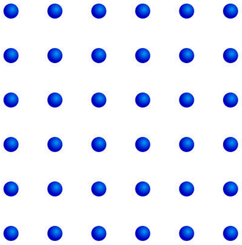

Atoms arrangement

Basic concept

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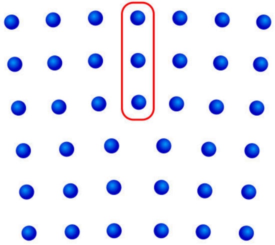

Insert a half atomic layer

(line in 2D, plane in 3D)

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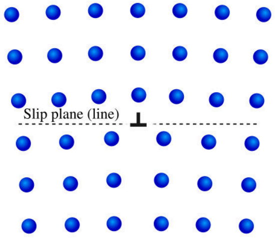

Obtain a dislocation defect

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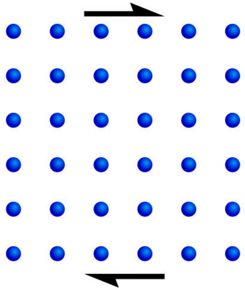

Another option: let's shear this lattice

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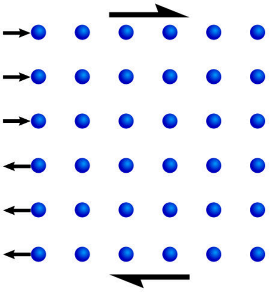

or rather push and pull along a particular plane

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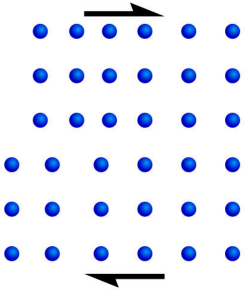

Shift (make a step on left side)

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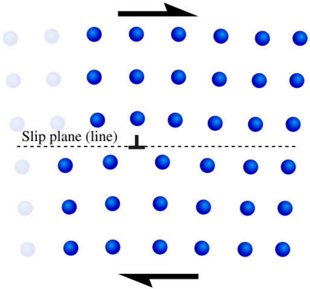

Of course the lattice deforms accordingly,
we can also imagine that we are far from free surfaces
(add transparent atoms)

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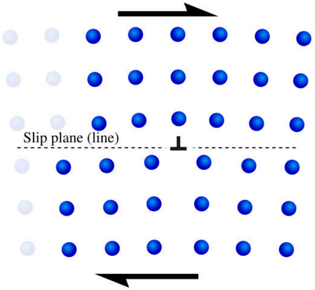

Let's shear more

or we might keep the same shear and wait until thermal fluctuations of atoms make the dislocation to step one step further

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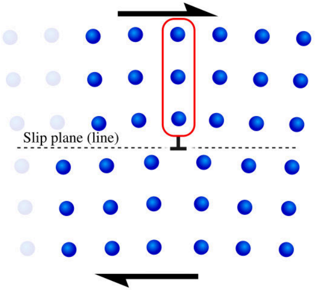

It has just make one more step

The configuration is equivalent as if we introduced a half atomic layer

Basic concept

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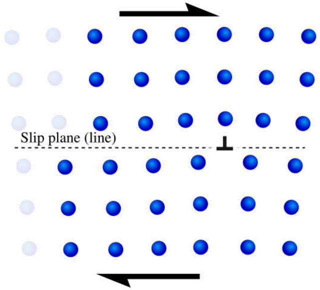

Another step

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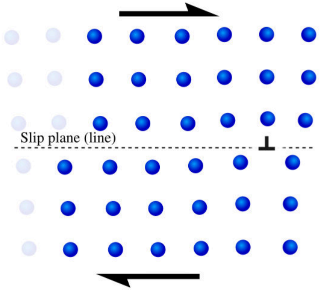

One more

Basic concept

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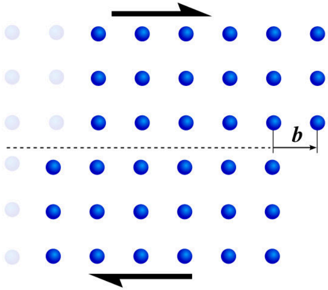
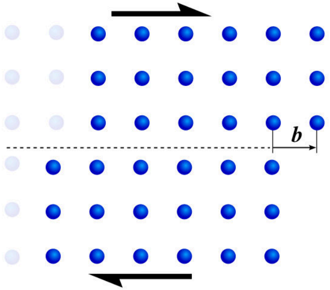


One more, and there is no more dislocations... but if we remove shear, an irreversible deformation remains in the system

Basic concept

- Dislocation is a line defect, a curve in a volume
- But the basics can be understood in 2D
- Carpet fold analogy



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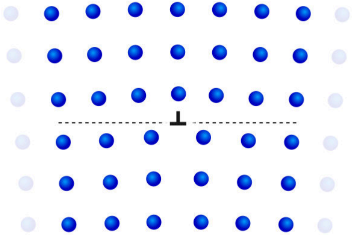
Dislocation in 2D: Peierls potential

- **Basics can be understood in 2D**
- Concept of an array of potential wells and energy barriers



Dislocation

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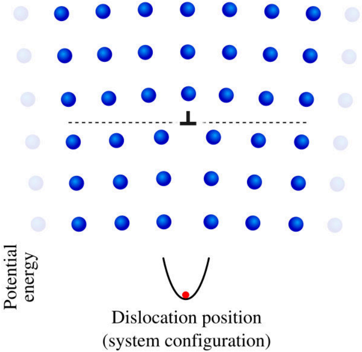

Dislocation in a stable equilibrium

Dislocation in 2D: Peierls potential

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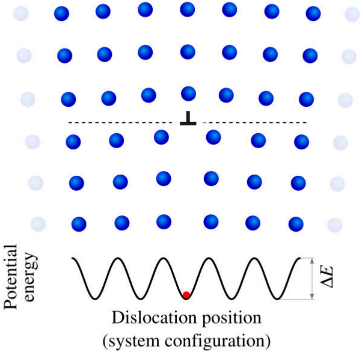

Array of potential wells and energy barriers

Dislocation in 2D: Peierls potential

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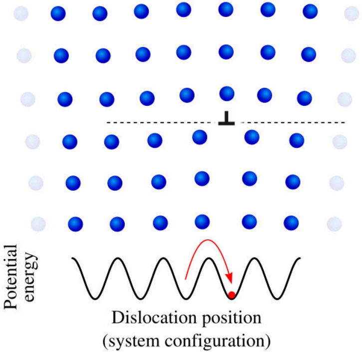

Jump to the right well

Dislocation in 2D: Peierls potential

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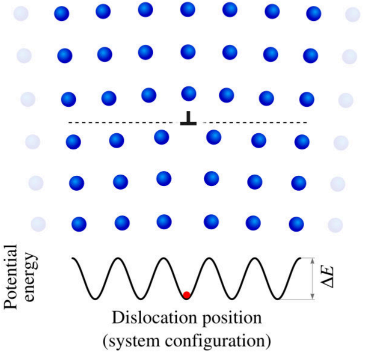

Array of potential wells and energy barriers (**Peierls potential**)

Dislocation in 2D: Peierls potential

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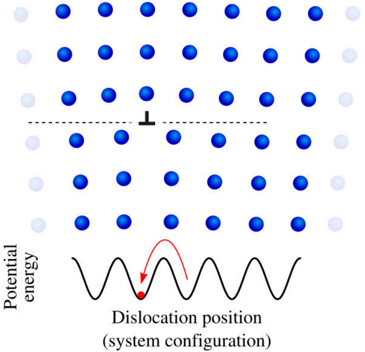

Jump to the left well

Dislocation in 2D: Peierls potential

- **Basics can be understood in 2D**
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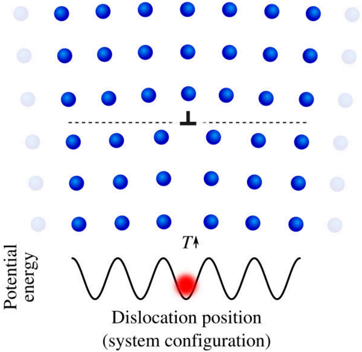
- Peierls potential
- Thermally activated motion



Increasing temperature $k_B T$ increases the probability of jump

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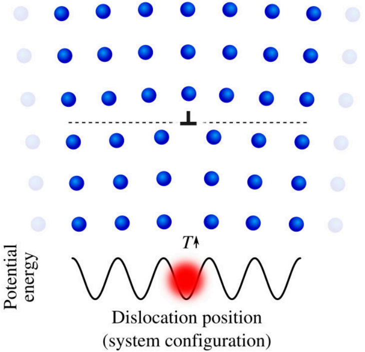

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Dislocation in 2D: Peierls potential

- **Basics can be understood in 2D**
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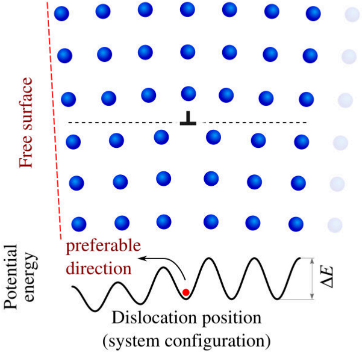
- Thermally activated motion
- Interaction with free surface



Near the free surface, an energetically faborable direction of motion is towards the surface

Dislocation in 2D: Peierls potential

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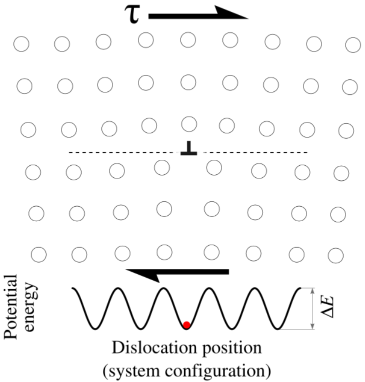

Shear loading

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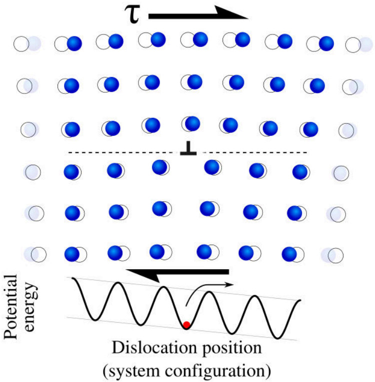
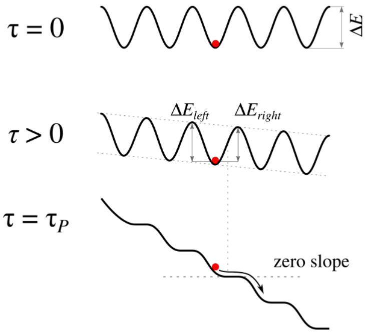


Shear loading bias the potential and dictates the favorable direction of motion

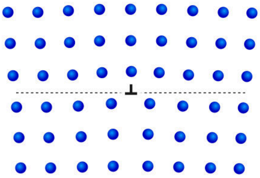
- **Basics can be understood in 2D**
- Concept of an array of potential wells and energy barriers
- Peierls potential
- Thermally activated motion
- Interaction with free surface
- Peierls stress

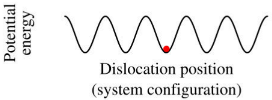


Increasing applied shear stress may result in a complete removing of the energy barrier (**Peierls stress** τ_P)

Dislocation in 2D: stress effects

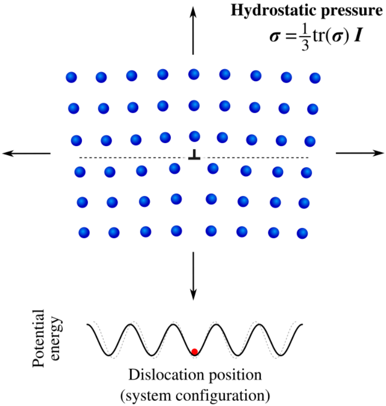
- **Basics can be understood in 2D**
- Applied stress affects dislocation motion





Dislocation

- **Basics can be understood in 2D**
- Applied stress affects dislocation motion
- Rather insensitive to hydrostatic pressure



Dislocation under hydrostatic pressure

Here $\mathrm{tr}(\sigma) > 0$

Dislocation in 2D: stress effects

- **Basics can be understood in 2D**
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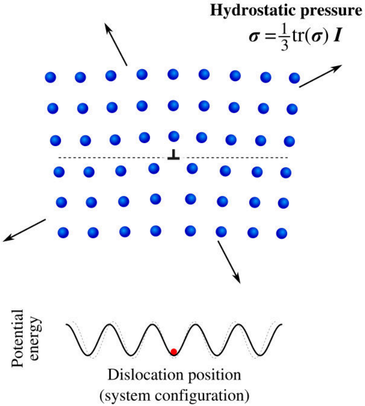

Dislocation under hydrostatic pressure

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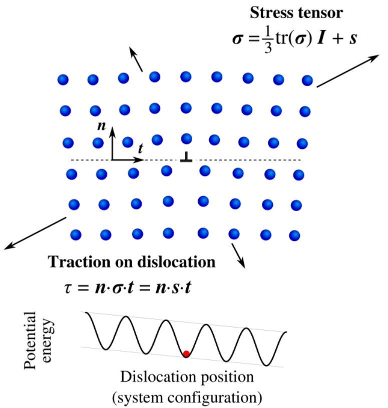
Dislocation in 2D: stress effects

- **Basics can be understood in 2D**
- Applied stress affects dislocation motion
- Rather insensitive to hydrostatic pressure
- Sensitive to the stress deviator



Dislocation is sensitive to the deviatoric part of the stress tensor $\boldsymbol{s} = \boldsymbol{\sigma} - \frac{1}{3}\mathrm{tr}(\boldsymbol{\sigma})\boldsymbol{I}$

$$\boxed{\tau = \boldsymbol{n}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{t} = \boldsymbol{n}\cdot\boldsymbol{s}\cdot\boldsymbol{t}}$$

Dislocation in 2D: stress effects

- **Basics can be understood in 2D**
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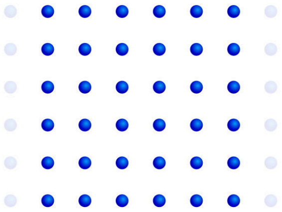
- Dislocation itself induces stresses



Perfect crystal

Dislocation in 2D: stress effects

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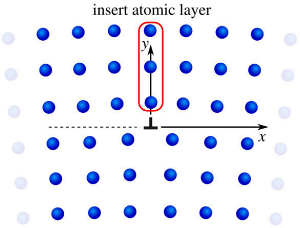

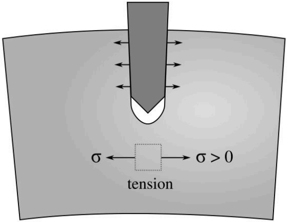

Dislocation: crystal with an **inserted layer** of atoms

Tensile stress below $y < 0 : \ \sigma_{xx} > 0$

Dislocation in 2D: stress effects

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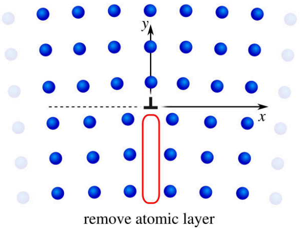

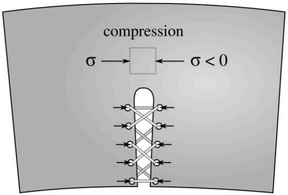

Dislocation: crystal with a **removed layer** of atoms

Compressive stress above $y > 0: \ \sigma_{xx} < 0$

Dislocation in 2D: stress effects

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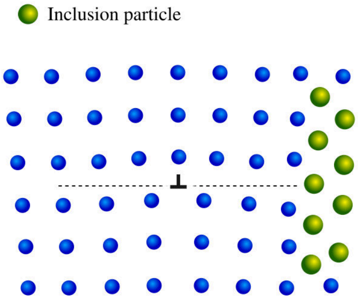
- Dislocation itself induces stresses
- Interactions with neighbouring defects: interstitial and vacancy defects



Inclusion on the glide line

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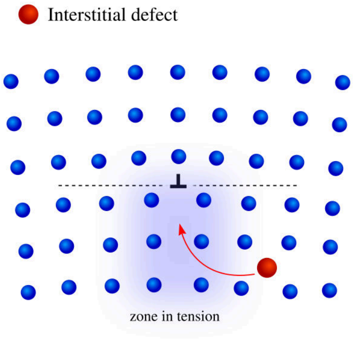

Interstitial defects migrate towards the zone of tensile stress induced by the dislocation

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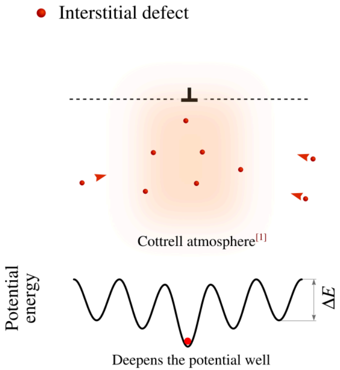

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[1] Cottrell & Bilby. Dislocation theory of yielding and strain ageing of iron. Proc Phys Soc A 62 (1949)

Dislocation in 2D: stress effects

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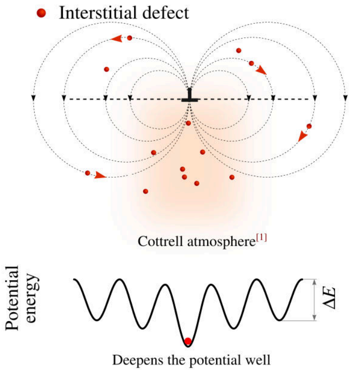

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Dislocation in 2D: stress effects

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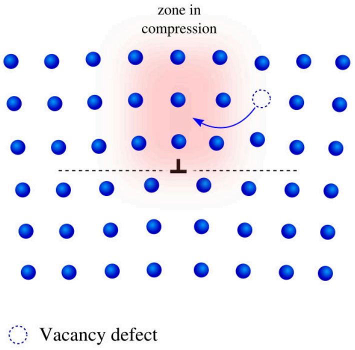

Vacancy defects migrate towards the zone of compressive stress induced by the dislocation

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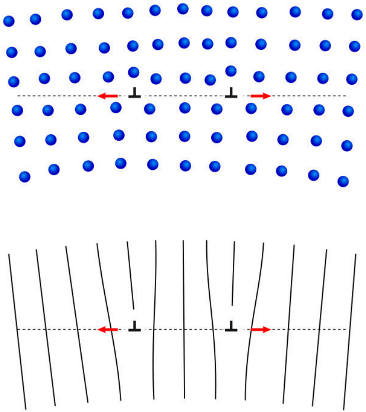
- Dislocation itself induces stresses
- Interactions with neighbouring defects: interstitial and vacancy defects
- Interactions between dislocations



Interaction of two “up” dislocations is repulsive

Dislocation in 2D: stress effects

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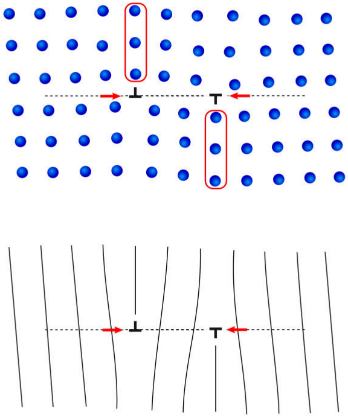
- Interactions with neighbouring defects: interstitial and vacancy defects
- Interactions between dislocations



Interaction of “up” and “down” dislocations is attractive and leads to annihilation of both defects

3D lattices

- Basics can be understood in 2D
- **But the complete picture can be drawn only in 3D**
- Crystallographic lattices in 3D:
  - • primitive cubic (pcc)
    (very rare for pure metals, *Po*)
  - • body-centered (bcc)
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  \+ and 10 other bravais lattices.
- Slip planes $\boldsymbol{n} = (ijk)$ (often the most densely packed)
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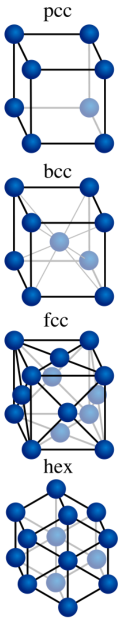
  $(\boldsymbol{n} \cdot \boldsymbol{d} = ip + jr + ks = 0)$



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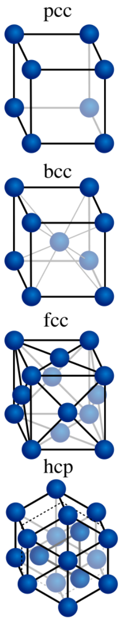

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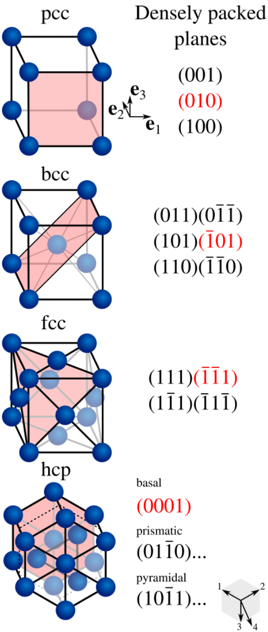

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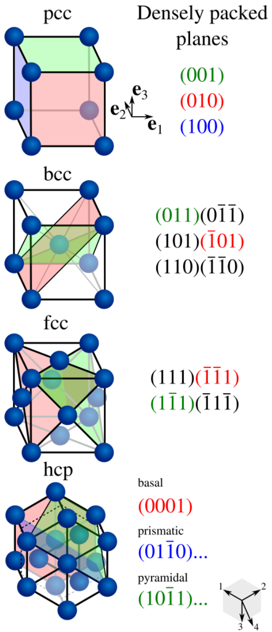

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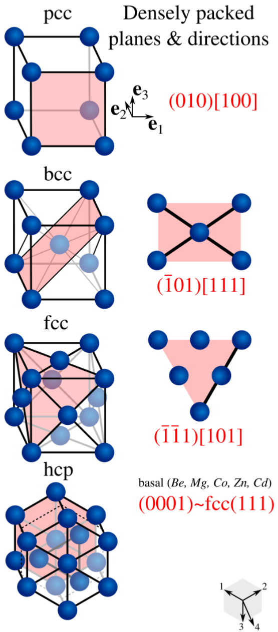

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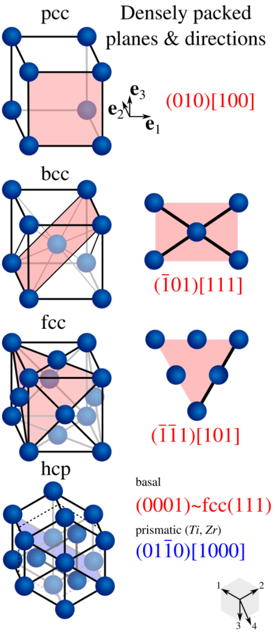
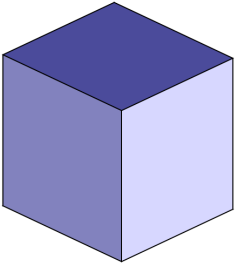


3D dislocations

- Slip plane $\boldsymbol{n}$
- Oriented dislocation line ξ
- Burgers vector $\boldsymbol{b}$
  can be expressed in terms of minimal distance between atoms in the slip system
- Dislocation types:
  - edge *(coin)*: $\boldsymbol{b}\cdot\xi = 0$
  - screw *(vis)*: $\boldsymbol{b}\times\xi = 0, \quad \forall \boldsymbol{n}$
  - mixed
- Burgers circuit
  provides the total Burgers vector within a contour
  Attention: $\boldsymbol{b}_\Gamma = 0$ *does not imply that there is no dislocations*



Box

- Slip plane $\boldsymbol{n}$
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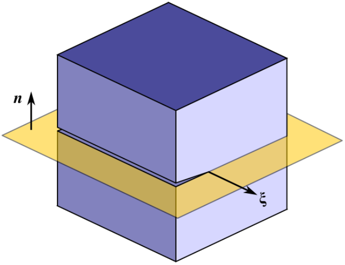

Introduce a cut along a densely packed plane with normal $\boldsymbol{n}$ (e.g. (111) in fcc)

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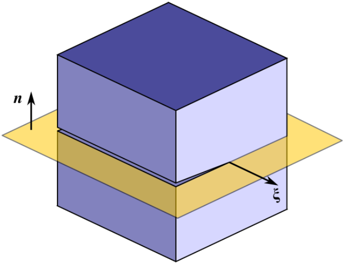

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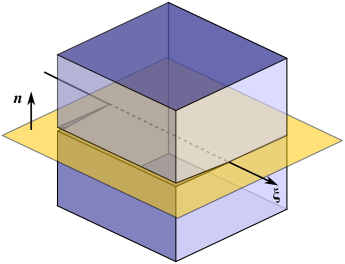

Cut's edge is the dislocation line, introduce an orientation $\boldsymbol{\xi}$

3D dislocations

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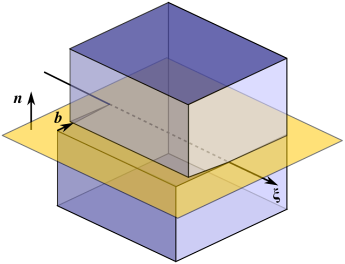

Shift the cut by a vector $\boldsymbol{b}$ along the plane **orthogonally** to the dislocation line and glue sides

Edge dislocation

3D dislocations

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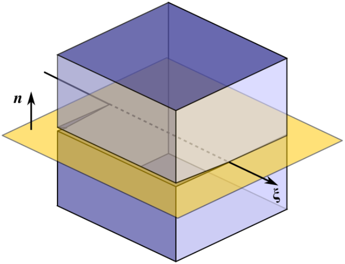

Cut in the box

3D dislocations

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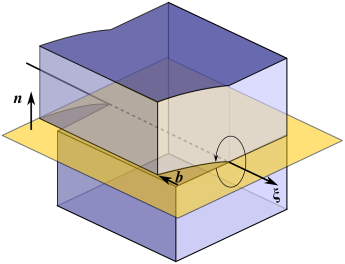

Shift the cut by a vector $\boldsymbol{b}$ along the plane **parallel** to the dislocation line and glue sides

Screw dislocation

3D dislocations

- Slip plane $\boldsymbol{n}$
- Oriented dislocation line $\boldsymbol{\xi}$
- Burgers vector $\boldsymbol{b}$
  can be expressed in terms of minimal distance between atoms in the slip system
- Dislocation types:
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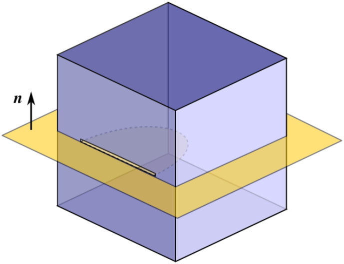

Semi-circular cut in the box

- Slip plane $\boldsymbol{n}$
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- Burgers vector $\boldsymbol{b}$
  can be expressed in terms of minimal distance between atoms in the slip system
- Dislocation types:
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  - mixed
- Burgers circuit
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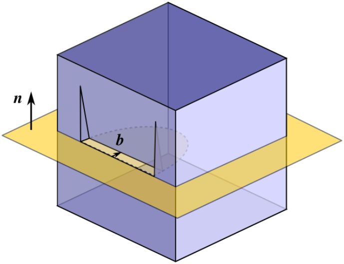

Shift the cut by a vector $\boldsymbol{b}$ and obtain a complex dislocation combining **screw and edge** dislocations

3D dislocations

- Slip plane $\boldsymbol{n}$
- Oriented dislocation line $\boldsymbol{\xi}$
- Burgers vector $\boldsymbol{b}$
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  - mixed
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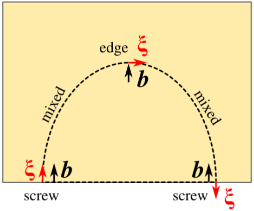

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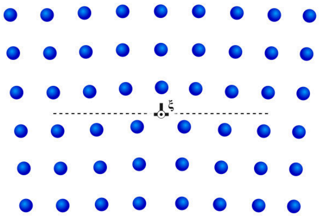

Edge dislocation

3D dislocations

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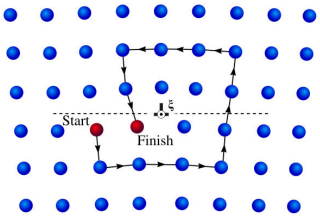

1 down, 3 right, 3 up, 3 left, 2 down

Make a contour around (right-hand rule *la règle de la main droite*)

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- Oriented dislocation line ξ
- Burgers vector $\boldsymbol{b}$
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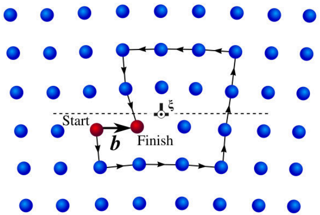

1 down, 3 right, 3 up, 3 left, 2 down

Make a contour around (right-hand rule *la règle de la main droite*), compute the net Burgers vector

3D dislocations

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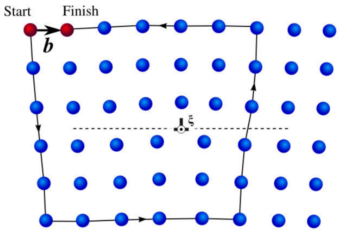

5 down, 5 right, 5 up, 5 left

Change the contour

3D dislocations

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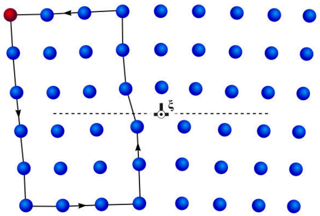

5 down, 3 right, 5 up, 3 left

Make a contour around a dislocation-free zone $\boldsymbol{b} = 0$

- Slip plane $\boldsymbol{n}$
- Oriented dislocation line ξ
- Burgers vector $\boldsymbol{b}$
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- Dislocation types:
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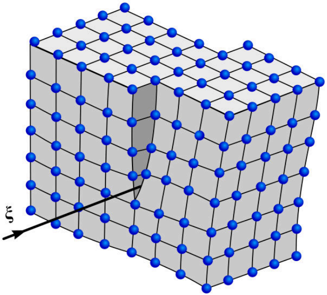

Screw dislocation

3D dislocations

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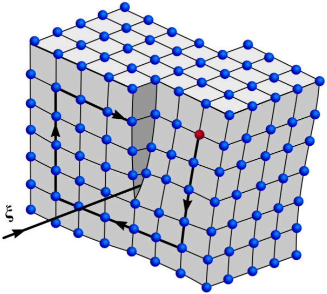

Draw a contour:
4 down, 5 left, 4 up, 3 right

- Slip plane $\boldsymbol{n}$
- Oriented dislocation line ξ
- Burgers vector $\boldsymbol{b}$
  can be expressed in terms of minimal distance between atoms in the slip system
- Dislocation types:
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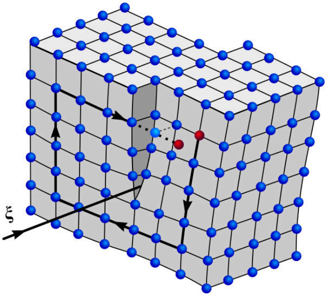

Draw a contour:
4 down, 5 left, 4 up, 3+2 right

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- Oriented dislocation line ξ
- Burgers vector $\boldsymbol{b}$
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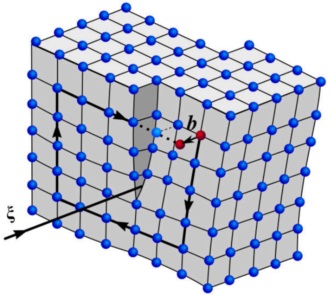
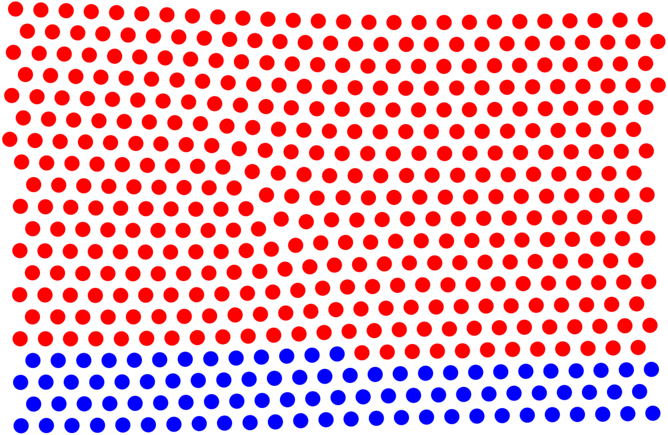


The Burgers vector is collinear with the dislocation line
$\boldsymbol{b} \parallel \xi$

Burgers curcuit example

Example from the Monday lecture on Molecular dynamics



Burgers curcuit example

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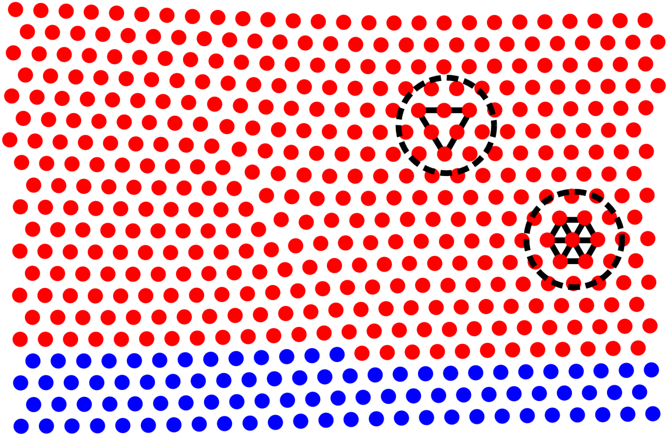
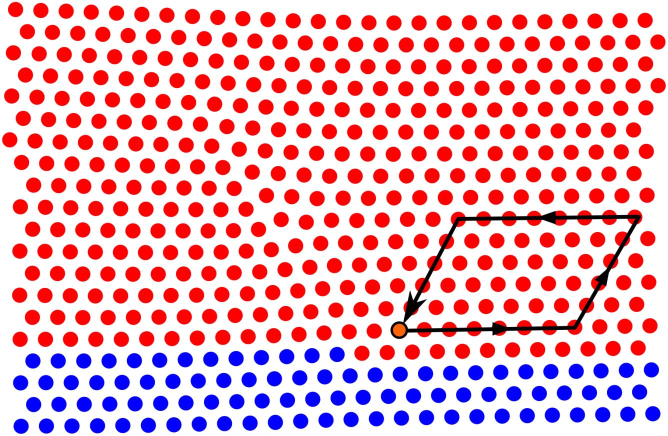


Basal hcp (0001) or fcc slip plane (111)

Burgers curcuit example

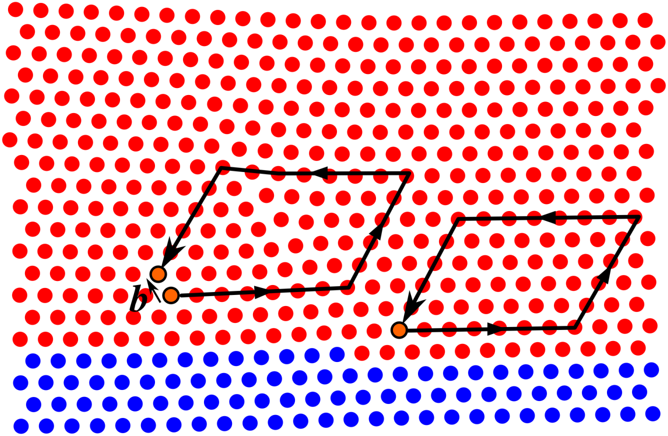
Example from the Monday lecture on Molecular dynamics



Contour 1: $\boldsymbol{b} = 0$

Burgers curcuit example

Example from the Monday lecture on Molecular dynamics



Contour 2: $\boldsymbol{b} = \frac{a}{\sqrt{2}}[\bar{1}10]$

Burgers curcuit example

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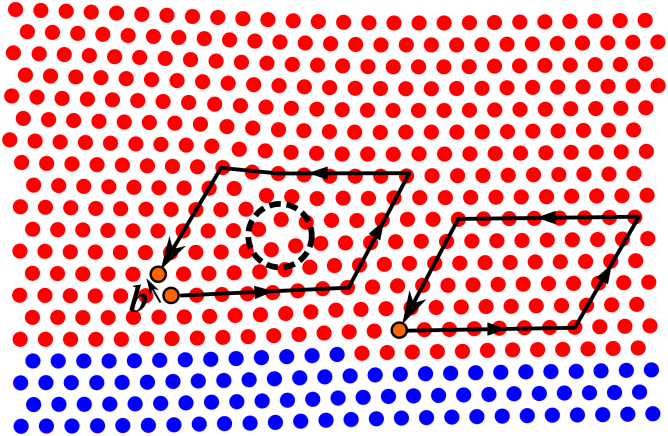

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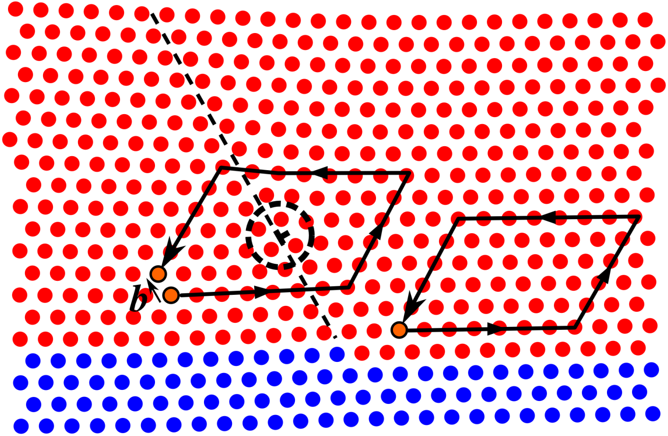


Contour 2: $\boldsymbol{b} = \frac{a}{\sqrt{2}}[\bar{1}10]$

Forces on dislocations

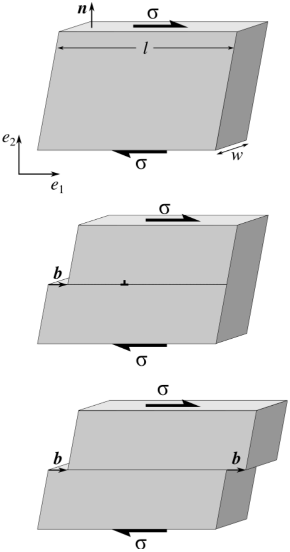
- A uniform stress $\boldsymbol{\sigma}$ shears a single crystal
- Force on the top $\boldsymbol{f} = \int \boldsymbol{\sigma} \cdot \boldsymbol{n} dA = \boldsymbol{\sigma}_n wl$
- Work of this force on shearing the crystal by amount $\boldsymbol{b} = \boldsymbol{e}_1|\boldsymbol{b}|$:

  $W = \boldsymbol{f} \cdot \boldsymbol{b} = wl\boldsymbol{\sigma}_n \cdot \boldsymbol{b}$
- At the same time dislocation of length w moves the distance l
- The "virtual" force $\boldsymbol{f}$ acting on the dislocation makes the same work:
  $wl\boldsymbol{f}\boldsymbol{e}_1 = W = wl\boldsymbol{\sigma}_n \cdot \boldsymbol{b}$ so

  $$\boldsymbol{f} = (\boldsymbol{\sigma}_n \cdot \boldsymbol{b})\boldsymbol{e}_1$$
- More generally (valid for edge and screw dislocations)

$$\boxed{\boldsymbol{f} = (\boldsymbol{\sigma} \cdot \boldsymbol{b}) \times \boldsymbol{\xi}}$$

(Peach-Koehler force)



Forces on dislocations

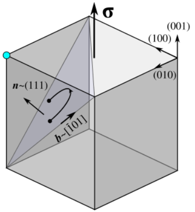
- Example: Frank-Read source in (111) plane with $\boldsymbol{b} \sim [0\bar{1}1]$, e.g. $\boldsymbol{b} = \frac{a}{2\sqrt{2}}(\boldsymbol{e}_3 - \boldsymbol{e}_1)$
- The box with this dislocation is under a unixial tension $\boldsymbol{\sigma} = \sigma \boldsymbol{e}_3 \otimes \boldsymbol{e}_3$
- Let's compute the Peach-Koehler force as

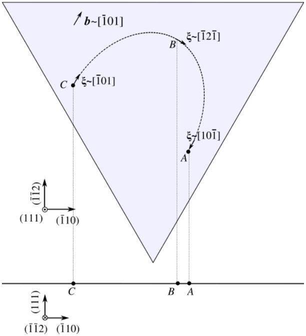
$$\boldsymbol{f} = (\boldsymbol{\sigma} \cdot \boldsymbol{b}) \times \boldsymbol{\xi}$$

- Where $\boldsymbol{\sigma} \cdot \boldsymbol{b} = \sigma \frac{a}{2\sqrt{2}} \boldsymbol{e}_3$
- At A: $\boldsymbol{\xi} = \frac{dl}{\sqrt{2}}(\boldsymbol{e}_1 - \boldsymbol{e}_3)$, $\boxed{d\boldsymbol{f} = \sigma \frac{a}{4} \boldsymbol{e}_2 dl}$

at B: $\boldsymbol{\xi} = \frac{dl}{\sqrt{2}}(2\boldsymbol{e}_2 - \boldsymbol{e}_1 - \boldsymbol{e}_3)$, $\boxed{d\boldsymbol{f} = -\sigma \frac{a}{4} (\boldsymbol{e}_1 + \boldsymbol{e}_2) dl}$

at C: $\boldsymbol{\xi} = \frac{dl}{\sqrt{2}}(\boldsymbol{e}_3 - \boldsymbol{e}_1)$, $\boxed{d\boldsymbol{f} = -\sigma \frac{a}{4} \boldsymbol{e}_2 dl}$





Note: line tension and self-interaction are not considered

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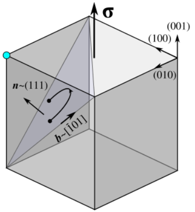

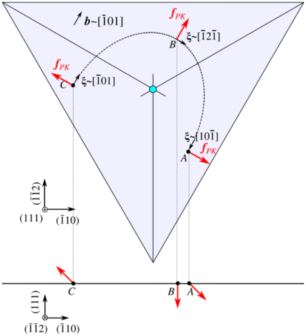

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Forces on dislocations

- Apart from the external load, dislocation has a **line tension** [J/m]
- Elastic energy per unit length stored around a dislocation (screw or edge)

$$E = \alpha\mu b^2, \quad \alpha \approx 0.5 - 1$$

- Line tension acting along the dislocation line is

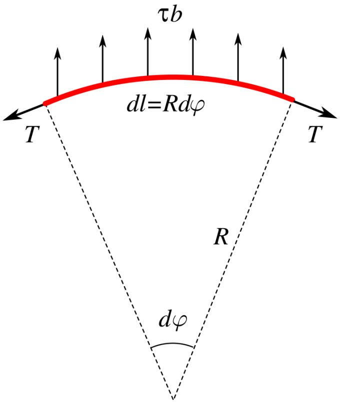
$$\boxed{T = \alpha\mu b^2}$$

- Then for a curved dislocation of radius R:

$$T d\phi = \tau b dl = \tau b R d\phi$$

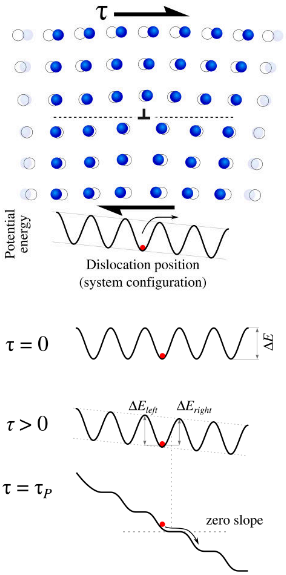
- For equilibrium (to keep this dislocation curved)

$$\tau = \alpha\mu b/R$$



Dislocation motion

- Recall the 2D case
- But dislocations are not point defect



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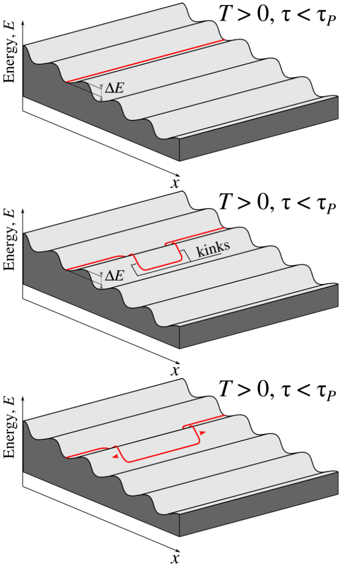
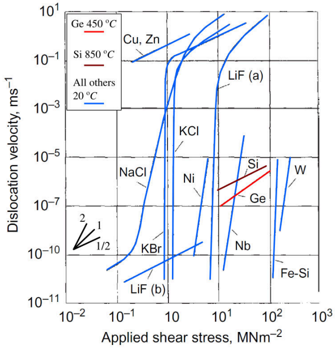


Dislocation motion

- Recall the 2D case
- But dislocations are not point defect
- When the resolved shear τ is smaller than the Peierls stress τ_P, thermally activated motion propagate via **kinks**
- When $\tau > \tau_P$, dislocations glide in "viscous drag" regime, where dislocation velocity is proportional to the force as well as the lattice friction

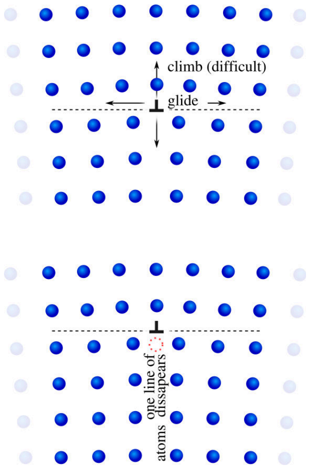
$$v_{\text{dis}} \sim f_{PK}, \quad f_{fr} \sim -g(T)v_{\text{dis}}$$

- Friction force f_{fr} comes from thermal vibrations of the lattice (phonons)
- In FCC: often viscous drag regime
- In BCC: viscous drag for edge and kinks-mechanism for screw



Velocity wrt the applied shear stress
Adapted from
P. Haasen. Physical Metallurgy, Cambridge University Press (1996)

- Note that the Peach-Koehler force is not necessarily in the slip plane $f_{PK} \cdot n \neq 0$
- Glide vs climb
- For edge dislocations:
  glide conserves the number of atoms,
  climb requires removing or adding lines of atoms (via, e.g. vacancies)
- Edge dislocations rather glide than climb at low temperature
- Very anisotropic motion
- Screw dislocation does not stick to a unique glide plane as $b \parallel \xi$
- Change of plane by screw dislocations results in **cross-slip**



Climb of screw dislocations requires addition or removal of atoms

Dislocation motion II

- Note that the Peach-Koehler force is not necessarily in the slip plane $\boldsymbol{f}_{PK} \cdot \boldsymbol{n} \neq 0$
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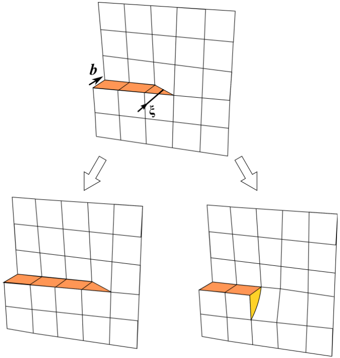

Screw dislocation may change the plane

Dislocation motion II

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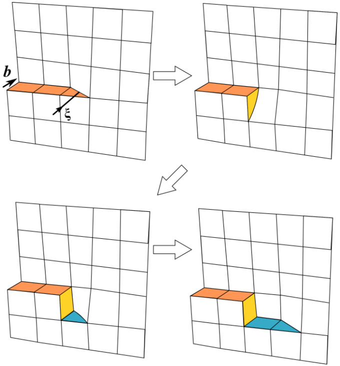
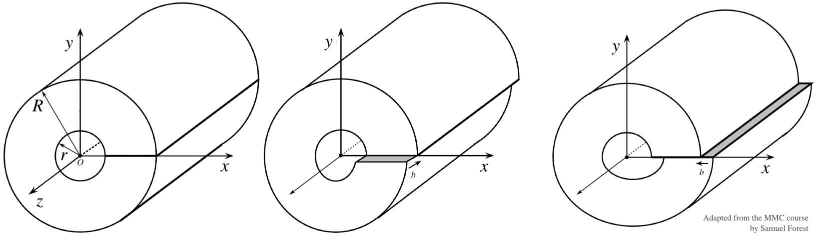


Cross-slip (imagine the remaining dislocation line)

Dislocation-induced stress field

- Volterra dislocation[1]



- Screw dislocation

$$\sigma_{xz} = -\frac{\mu b}{2\pi}\frac{y}{(x^2+y^2)}$$
$$\sigma_{yz} = \frac{\mu b}{2\pi}\frac{x}{(x^2+y^2)}$$

- Edge dislocation

$$\sigma_{xx} = -\frac{\mu b}{2\pi(1-\nu)}\frac{y(3x^2+y^2)}{(x^2+y^2)^2}$$
$$\sigma_{yy} = \frac{\mu b}{2\pi(1-\nu)}\frac{y(x^2-y^2)}{(x^2+y^2)^2}$$
$$\sigma_{xy} = -\frac{\mu b}{2\pi(1-\nu)}\frac{x(x^2-y^2)}{(x^2+y^2)^2}$$
$$\sigma_{zz} = \nu(\sigma_{xx}+\sigma_{yy})$$

[1] Volterra V. Sur l'équilibre des corps élastiques multiplement connexes. Annal. Sci. de l'Ecole Norm. Supér. 24 (1907).

Dislocation-induced stress field

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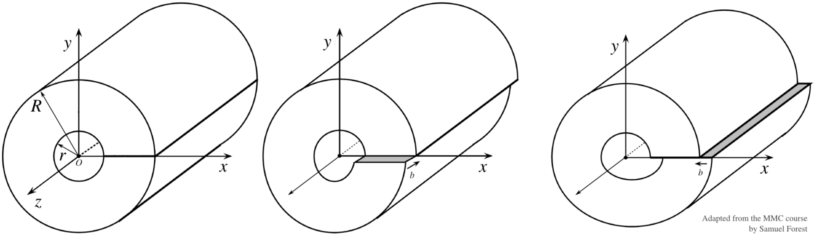

- Elastic energy per unit length for an edge and screw dislocation

$$E_e = \frac{\mu b^2}{4\pi(1-\nu)} \ln(R/r), \quad E_s = \frac{\mu b^2}{4\pi} \ln(R/r)$$

- For a mixed dislocation (edge $b\sin(\theta)$, screw $b\cos(\theta)$)

$$E(\theta) = \frac{\mu b^2(1-\nu\cos^2(\theta))}{4\pi(1-\nu)} \ln(R/r) \approx \alpha\mu b^2, \quad \alpha \approx 0.5 - 1$$

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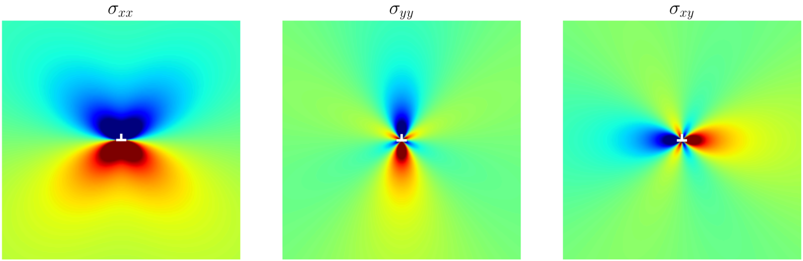
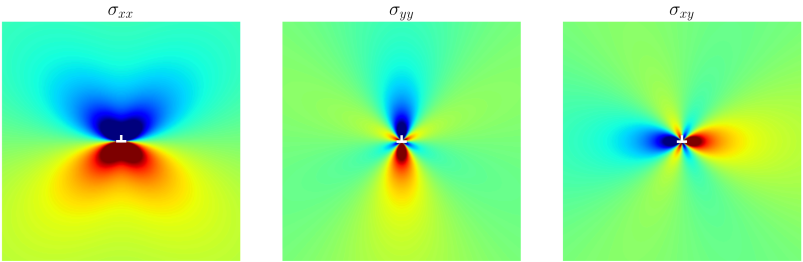
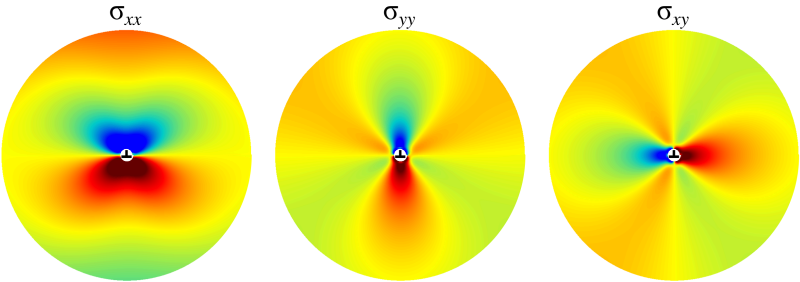


Theoretical stress field

Dislocation-induced stress field

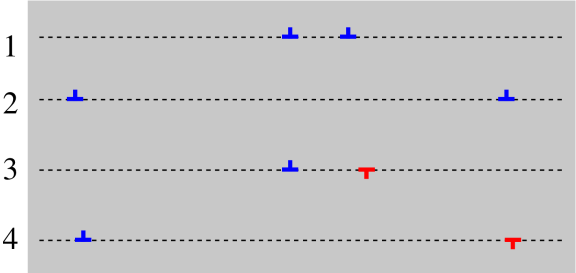




Comparison with the finite element solution

Interaction between dislocations

- Interaction between two edge **dislocations on the same line**
- Dislocations of the same sign repeal because:
  - when close $E \approx \mu(2b)^2$
  - when far $E \approx 2\mu(b)^2$
- Dislocations of opprosite sign attract because:
  - when close $E \approx \mu(b-b)^2 = 0$
  - when far $E \approx 2\mu(b)^2$



Interaction between dislocations

- Interaction between two edge **dislocations on parallel lines**
- Interaction energy is the work done by the stress field induced by 1 on displacing 2:

$$E_{\text{inter}} = \int_x^{\infty} (\sigma_{xy} b_x + \sigma_{yy} b_y + \sigma_{yz} b_z) dx = -\int_y^{\infty} (\sigma_{xx} b_x + \sigma_{xy} b_y + \sigma_{xz} b_z) dx$$

- The resulting forces for two parallel dislocation of the same sign $b_x^1 = b_x^2 = b$:

$$f_x = -\frac{\partial E_{\text{inter}}}{\partial x} = \frac{\mu b^2}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

$$f_y = -\frac{\partial E_{\text{inter}}}{\partial y} = \frac{\mu b^2}{2\pi(1-\nu)} \frac{y(3x^2-y^2)}{(x^2+y^2)^2}$$

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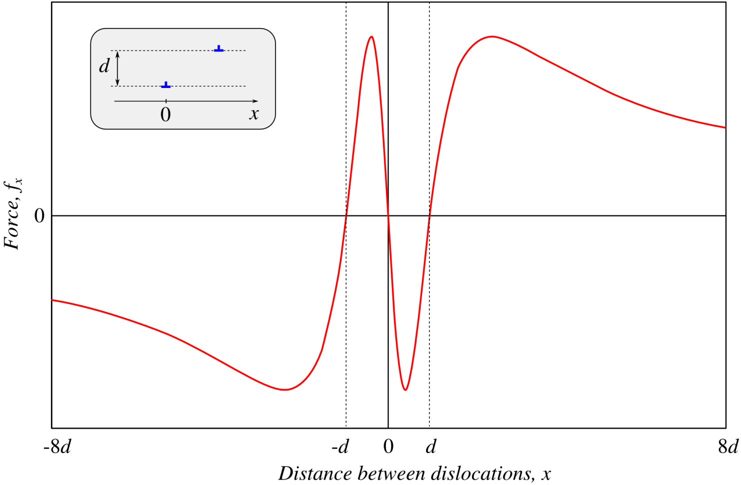

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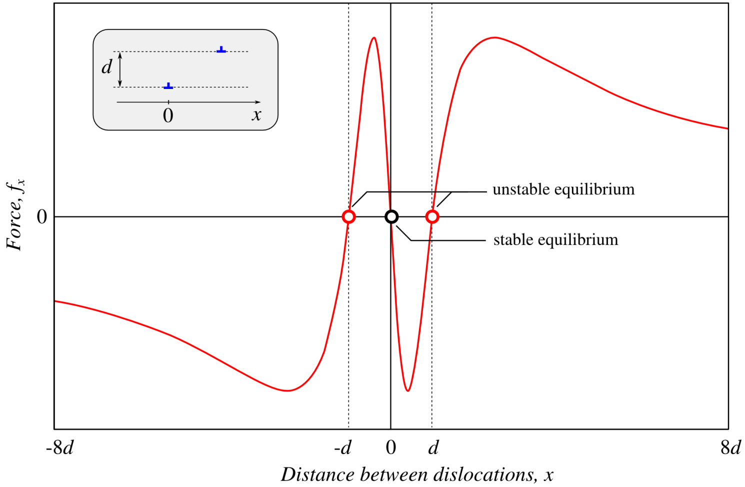

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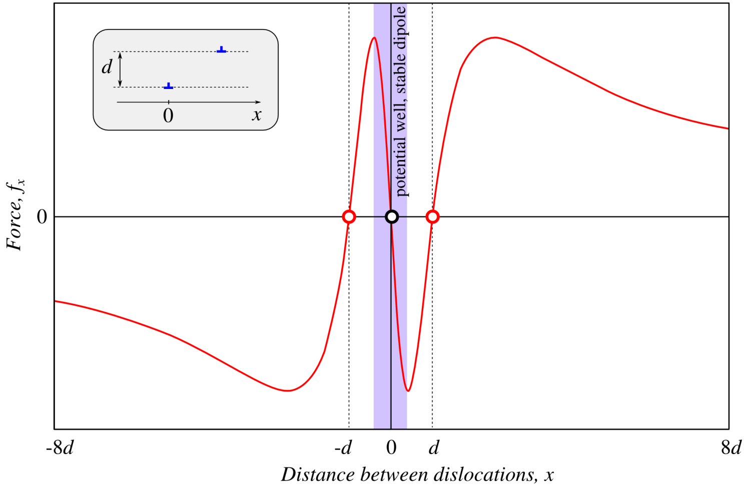

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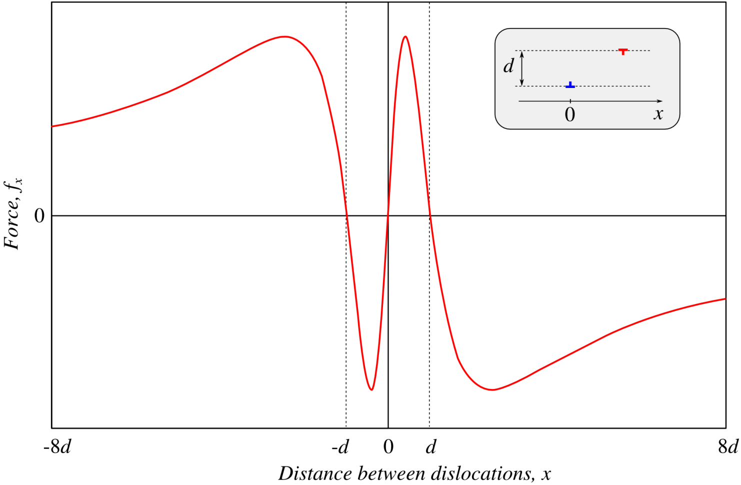

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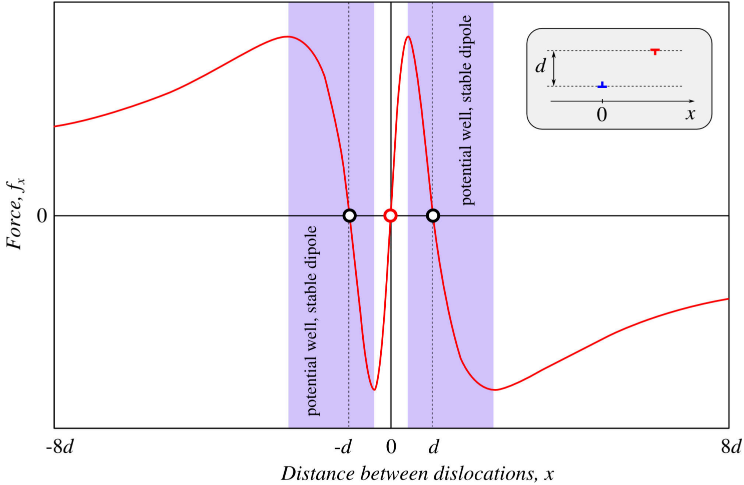

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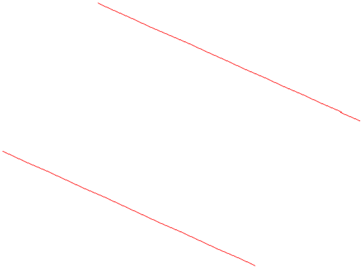

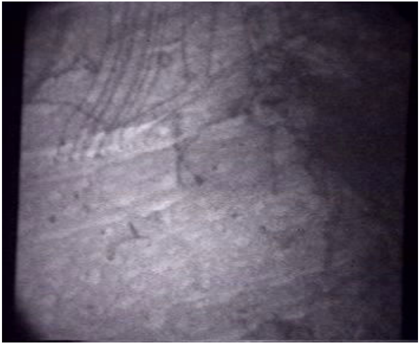

from Marc Fivel (SiMap, INP Grenoble), `www.numodis.fr/tridis`

Dislocations interact with the environment

- **Free surface** $\sigma \cdot n = 0$
- To ensure zero stress vector, introduce an "image dislocation" of the opposite sign at the same distance from the surface:

$$(\sigma^{\text{real}} + \sigma^{\text{imag}}) \cdot n = 0$$

- Dislocations of opposite sign on the same line **attract each other**
- Note: an additional energy is needed to brake the oxide film
- **Rigid wall** $u = 0$, repulsion
- **Rigid inclusions** do not let dislocations glide quietly

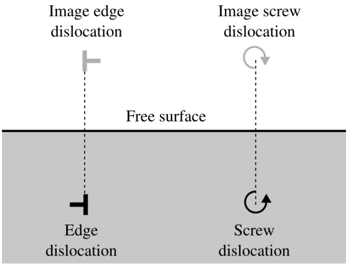

Image dislocation in air :)

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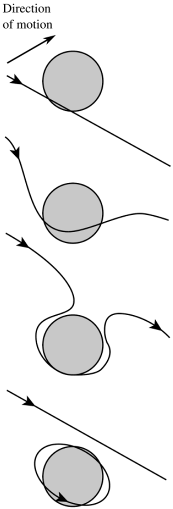

Interaction with a particle in dispersion-strengthened alloy
Orowan mechanism
Hirsch P.B., Humphreys F.J. Physics of Strength and Plasticity, Ed. A.S. Argon, MIT Press (1969)

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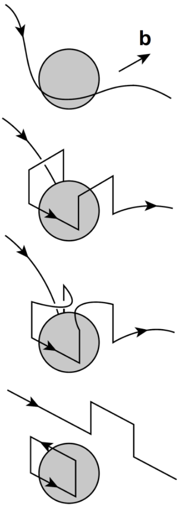

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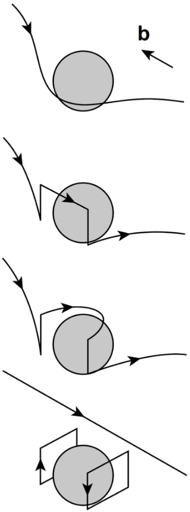

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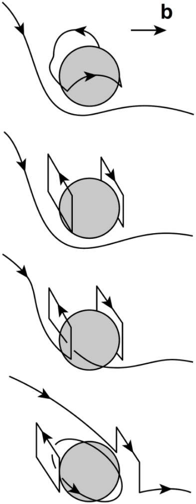

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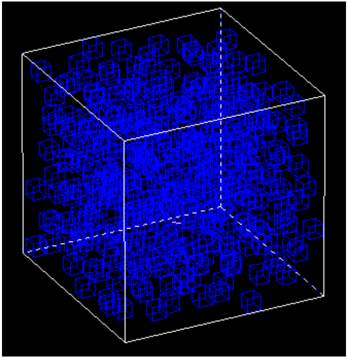

from Marc Fivel (SiMap, INP Grenoble),
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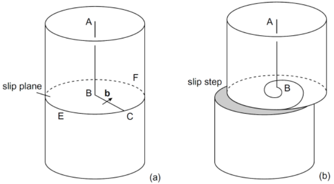
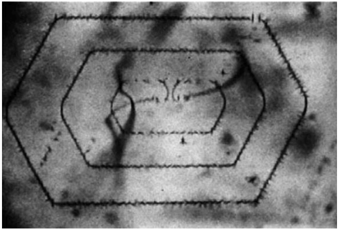
Origin of dislocations

- In virgin well-annealed crystal
  $\rho \approx 10^{10}\ \mathrm{m}^{-2}$
- At early stages of deformation: single set of parallel slip planes is active
- At large deformation: $\rho \approx 10^{15}\ \mathrm{m}^{-2}$, different slip systems are activated
- At lattice defects and due to stress concentrators
- At grain boundaries
- Frank-Read sources (double and single ended)
- From the free surface
- Geometrically necessary dislocations to accommodate indenter's form



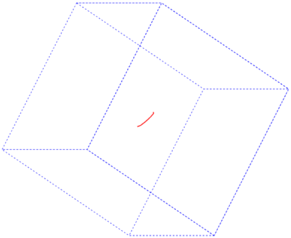
Single-ended Frank-Read source
from D. Hull, D.J. Bacon, Introduction to Dislocations, Elsevier (2011)



Double-ended Frank-Read source in silicon crystal
from Dash, Dislocation and Mechanical Properties of Crystals, Wiley (1957)

Origin of dislocations

- In virgin well-annealed crystal
  $\rho \approx 10^{10}$ m^{-2}
- At early stages of deformation: single set of parallel slip planes is active
- At large deformation: $\rho \approx 10^{15}$ m^{-2}, different slip systems are activated
- At lattice defects and due to stress concentrators
- At grain boundaries
- Frank-Read sources (double and single ended)
- From the free surface
- Geometrically necessary dislocations to accommodate indenter's form



DD simulation of double ended Frank-Read source in a cube-shaped box with rigid walls

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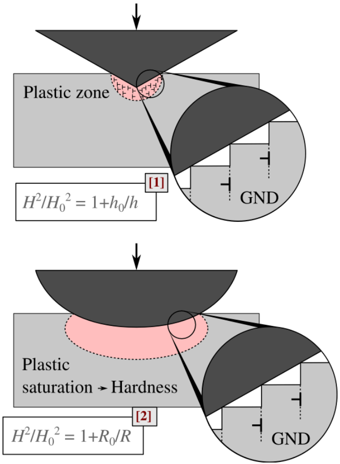


Size effect in nano-indentation due to geometrically necessary dislocations

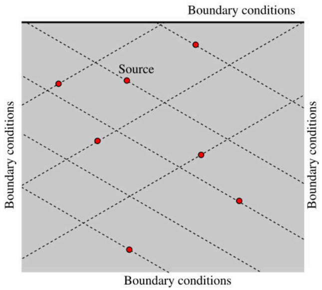
[1] Nix, Gao. J Mech Phys Solids (1998)
[2] Swadener, George, Pharr. J Mech Phys Solids (2002)

2D DD[1]

- Inifinite straight and parallel dislocations
- No line tension
- No topological changes and intersections

Ingredients

- Only edge dislocations (points) randomly distributed on discrete slip lines
- Randomly distributed sources with stress and distance threshold:
  $|f| > f_{nuc}$: generates $\pm b$ dislocations at distance: $l_n = \mu b/[2\pi(1-\nu)f_{nuc}]$
- On slip lines, randomly distributed obstacles with strength f^i_{obs}



R. Van der Giessen, A. Needleman. Discrete dislocation plasticity: a simple planar model. Model Sim Mater Sci Eng (1995)

Simulation of dislocations in 2D

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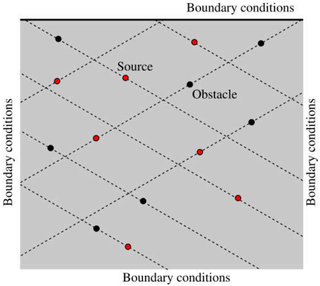

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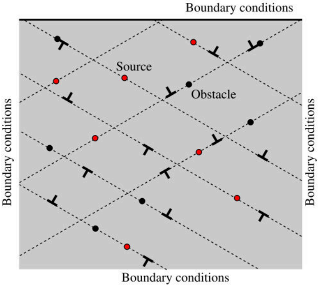

R. Van der Giessen, A. Needleman. Discrete dislocation plasticity: a simple planar model. Model Sim Mater Sci Eng (1995)

Algorithm

- Impose an external stress field $\boldsymbol{\sigma}^{ext}(x,y)$
- Find Peach-Koehler force on each source from external stress $\boldsymbol{f}_i^{ext}$ and from dislocations $\boldsymbol{f}_i^d$
- If $|\boldsymbol{f}_i^{ext} + \boldsymbol{f}_i^d| \geq f_{nuc}$: create $\pm b$ dislocations
- Compute forces on all dislocations
  $\boldsymbol{f}_j = -\sum \nabla_x E_{int}(\boldsymbol{x}_i, \boldsymbol{x}_j) + \boldsymbol{f}_i^{ext}$
- Assume linear relation between velocity and PK force:
  $\boldsymbol{f}_j = B\dot{\boldsymbol{x}}_j$
- Integrate in time *Euler-trapezoid method*:
  $\boldsymbol{x}_j^E(t+\Delta t) = \boldsymbol{x}_j(t) + \frac{1}{B}\boldsymbol{f}_j(\boldsymbol{x}(t))$
  $\boldsymbol{x}_j(t+\Delta t) = \boldsymbol{x}_j(t) + \frac{1}{2B}\left[\boldsymbol{f}_j(\boldsymbol{x}(t)) + \boldsymbol{f}_j(\boldsymbol{x}^E(t+\Delta t))\right]$

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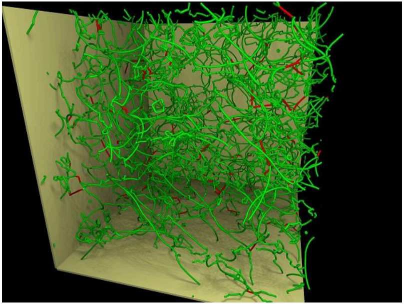
3D DD[1]

- Splines or edge/screw segments
- Glide and climb
- Arbitrary morphology of dislocations
- Topological changes and intersections
- Enhanced interaction with the material and boundaries



Ingredients

- Frank-Read sources
- Free-surface
- Grain boundaries
- Possible coupling with the FEM method and with MD both in 2D and 3D

Bulatov V.V., Cai W. Computer Simulations of Dislocations, Oxford University Press, 2006.

Algorithm

- Impose/compute via FEM a stress field $\boldsymbol{\sigma}^{ext}(x, y)$
- Use shape functions for positions and velocities:

  $\boldsymbol{r}(\xi, t) = N_i(\xi)\boldsymbol{r}_i(t) \quad \boldsymbol{v}(\xi, t) = N_i(\xi)\boldsymbol{v}_i(t)$
- Find Peach-Koehler force on each node from external stress $\boldsymbol{f}_i^{ext}$ and from all dislocation segments $\boldsymbol{f}_i^d = -\int_{Dj} \nabla_x E_{inter} d\Gamma$
- Assume over-damped dynamics, drag force is a linear (in simplest case) function of velocity:

  $\boldsymbol{f}_j^{drag} = -\boldsymbol{B} \cdot \boldsymbol{v}_j$
- Drag force cannot oppose everywhere the PK force, so it is satisfied in a weak sense:

  $\int_D N_i(-\boldsymbol{B} \cdot \boldsymbol{v}_j N_j + f^{PK}) dl = 0$
- Giving the linear system of equations:

  $\sum \boldsymbol{B}_{ij} \cdot \boldsymbol{v}_j = \boldsymbol{f}_i, \quad B_{ij} = \int_D -\boldsymbol{B} N_i N_j dl$
- Integrate in time *Euler-trapezoid method*:

  $\boldsymbol{x}_j^E(t + \Delta t) = \boldsymbol{x}_j(t) + \boldsymbol{v}_j(t)\Delta t$

  $\boldsymbol{x}_j(t + \Delta t) = \boldsymbol{x}_j(t) + \frac{1}{2}(\boldsymbol{v}_j(t) + \boldsymbol{v}_j^E(t + \Delta t))\Delta t$

Animations

www.numodis.fr/

optidis.gforge.inria.fr/videos/video.html

References

- D. Hull and D.J. Bacon. Introduction to Dislocations, Elsevier (2011)
- J.P. Hirth and J. Lothe. Theory of dislocations. (1982)
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- http://www.numodis.fr/

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Merci de votre attention !