Multiscale Simulations of Materials and Structures

Lecture 7.
Dislocation Dynamics

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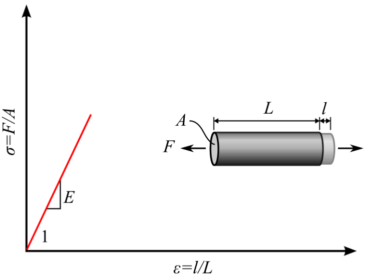
Outline

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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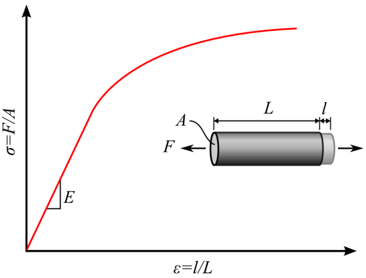

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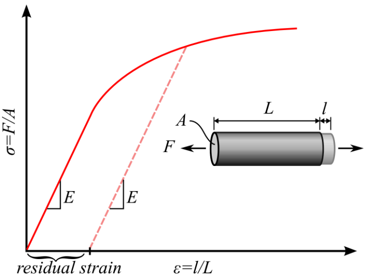

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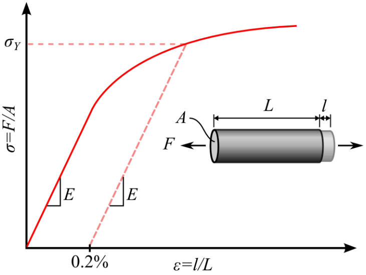

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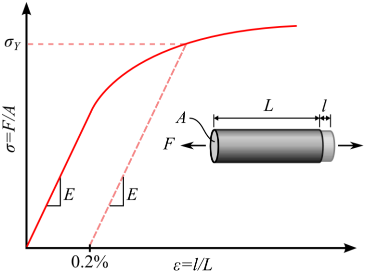
Introduction

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

Objective:

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



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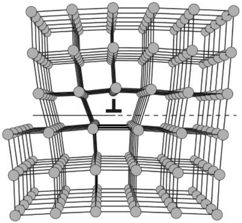
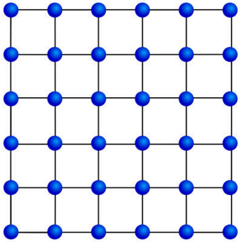


from

[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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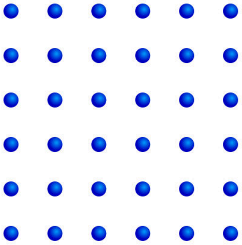

Atoms arrangement

Basic concept

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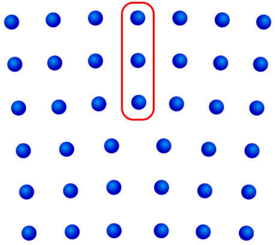

Insert a half atomic layer

(line in 2D, plane in 3D)

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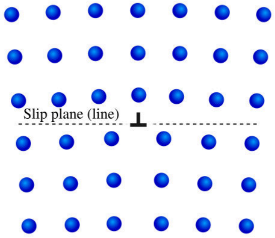

Obtain a dislocation defect

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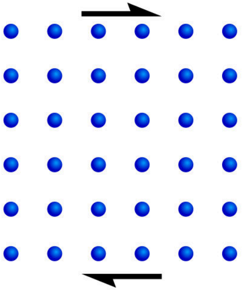

Another option: let's shear this lattice

Basic concept

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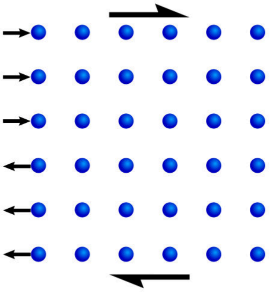

or rather push and pull along a particular plane

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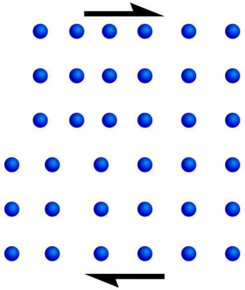

Shift (make a step on left side)

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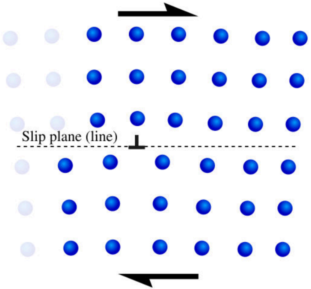

Of course the lattice deforms accordingly,

we can also imagine that we are far from free surfaces

(add transparent atoms)

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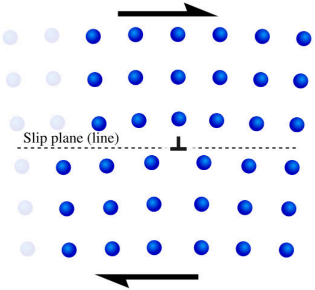

Let's shear more

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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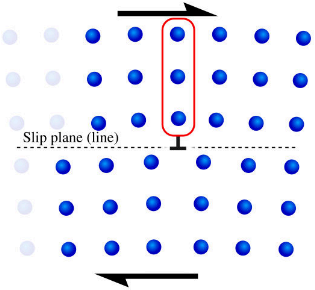

It has just make one more step

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

Basic concept

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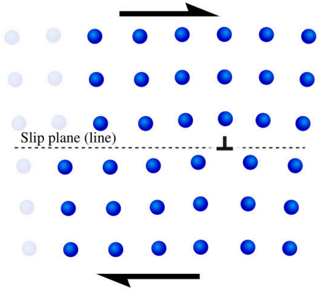

Another step

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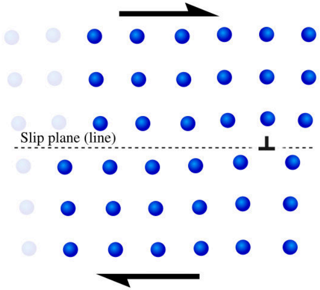

One more

Basic concept

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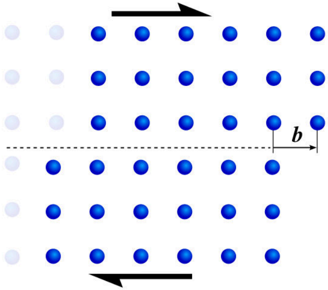
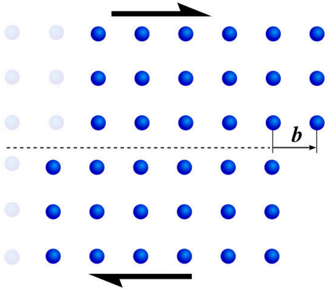


One more, and there is no more dislocations... but if we remove shear, an irreversible deformation remains in the system

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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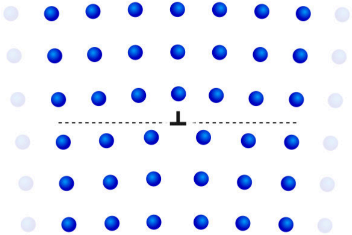
Dislocation in 2D: Peierls potential

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



Dislocation

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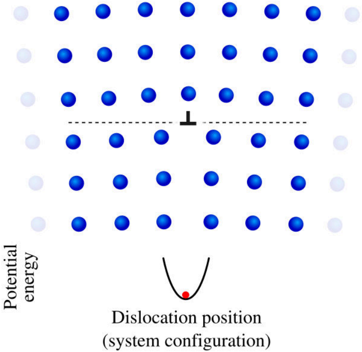

Dislocation in a stable equilibrium

Dislocation in 2D: Peierls potential

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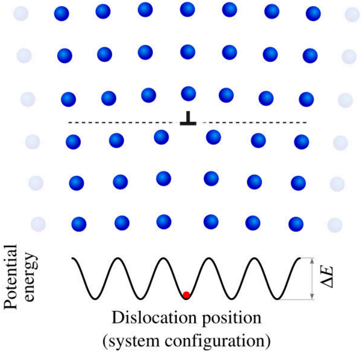

Array of potential wells and energy barriers

Dislocation in 2D: Peierls potential

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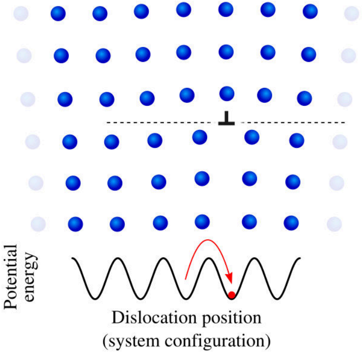

Jump to the right well

Dislocation in 2D: Peierls potential

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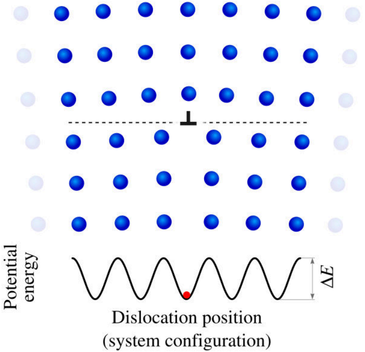

Array of potential wells and energy barriers (**Peierls potential**)

Dislocation in 2D: Peierls potential

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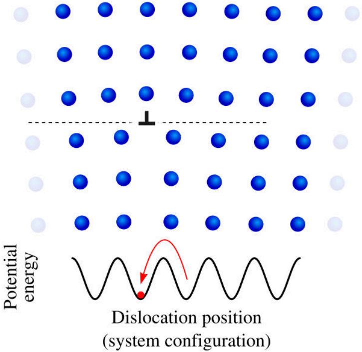
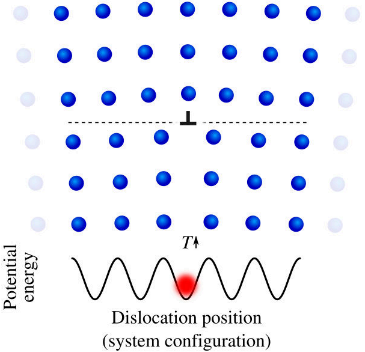


Jump to the left well

Dislocation in 2D: Peierls potential

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



Increasing temperature $k_B T$ increases the probability of jump

Dislocation in 2D: Peierls potential

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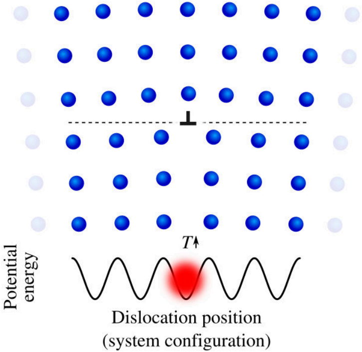

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Dislocation in 2D: Peierls potential

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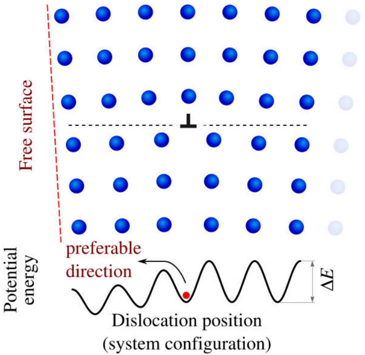
- Thermally activated motion
- Interaction with free surface



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

Dislocation in 2D: Peierls potential

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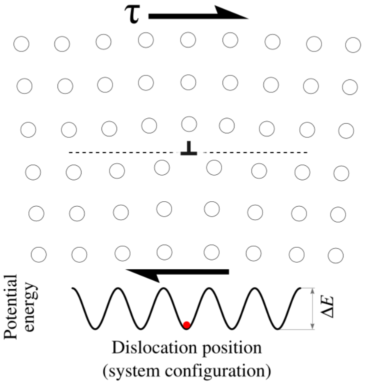

Shear loading

Dislocation in 2D: Peierls potential

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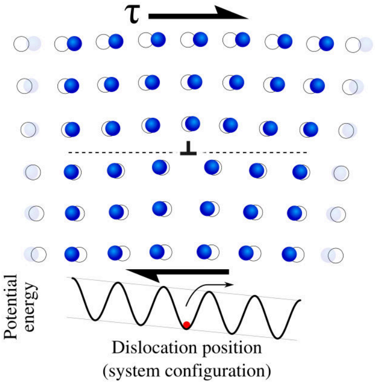

Shear loading bias the potential and dictates the favorable direction of motion

Dislocation in 2D: Peierls potential

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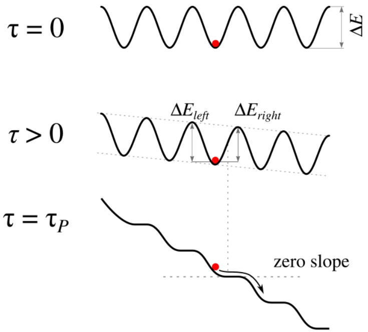
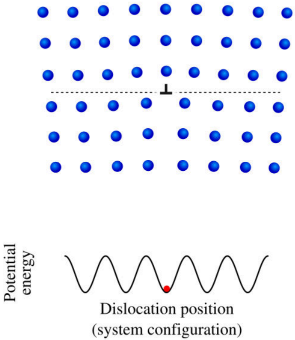
- Thermally activated motion
- Interaction with free surface
- Peierls stress



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

Dislocation in 2D: stress effects

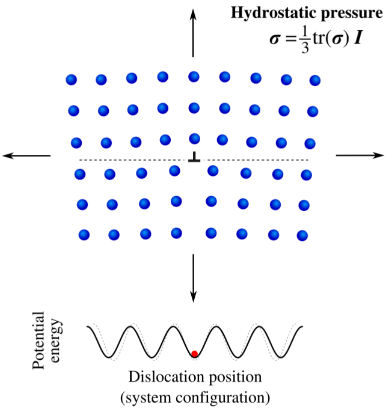
- **Basics can be understood in 2D**
- Applied stress affects dislocation motion



Dislocation

Dislocation in 2D: stress effects

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



Dislocation under hydrostatic pressure

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

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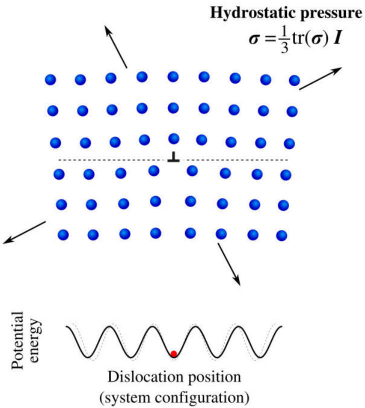

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Dislocation in 2D: stress effects

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- Applied stress affects dislocation motion
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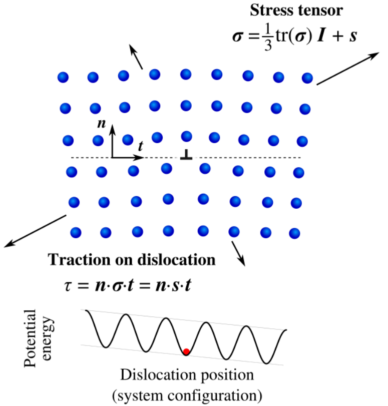
- Sensitive to the stress deviator



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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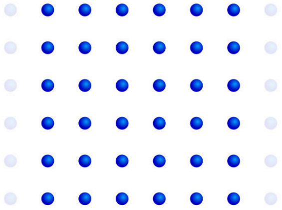
- Dislocation itself induces stresses



Perfect crystal

Dislocation in 2D: stress effects

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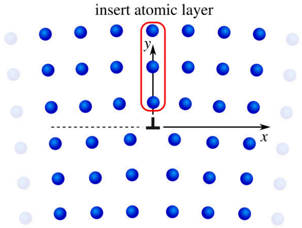

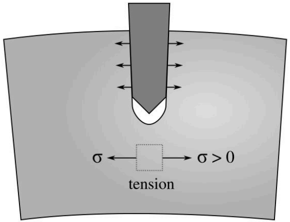

Dislocation: crystal with an **inserted layer** of atoms

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

Dislocation in 2D: stress effects

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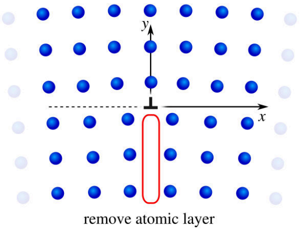

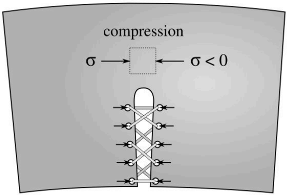

Dislocation: crystal with a **removed layer** of atoms

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

Dislocation in 2D: stress effects

- **Basics can be understood in 2D**
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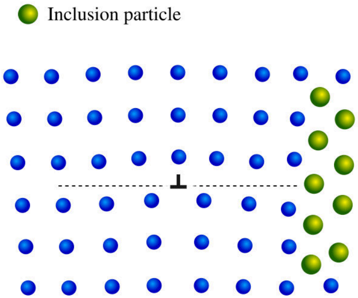
- Dislocation itself induces stresses
- Interactions with neighbouring defects: interstitial and vacancy defects



Inclusion on the glide line

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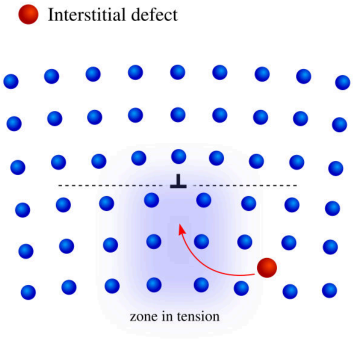

Interstitial defects migrate towards the zone of tensile stress induced by the dislocation

Dislocation in 2D: stress effects

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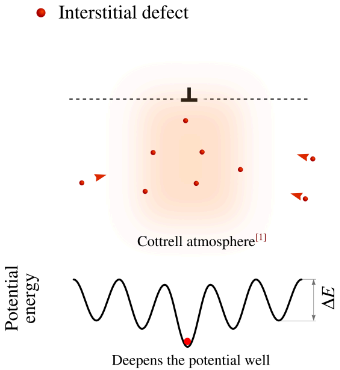

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[1] Cottrell & Bilby. Dislocation theory of yielding and strain ageing of iron. Proc Phys Soc A 62 (1949)

Dislocation in 2D: stress effects

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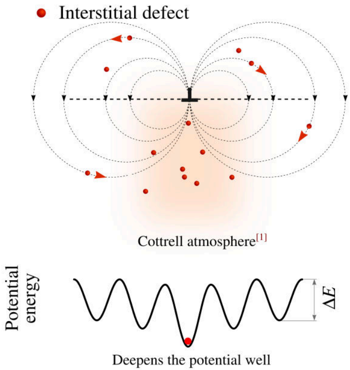

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Dislocation in 2D: stress effects

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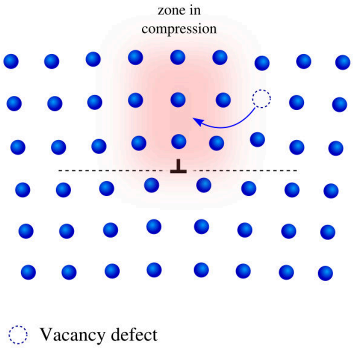

Vacancy defects migrate towards the zone of compressive stress induced by the dislocation

Dislocation in 2D: stress effects

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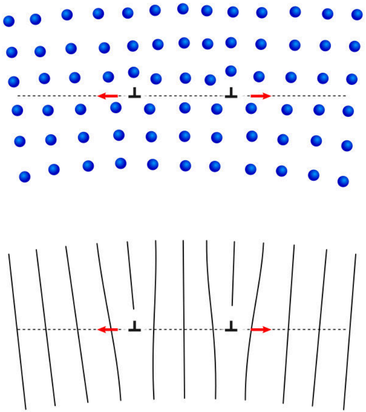
- Dislocation itself induces stresses
- Interactions with neighbouring defects: interstitial and vacancy defects
- Interactions between dislocations



Interaction of two “up” dislocations is repulsive

Dislocation in 2D: stress effects

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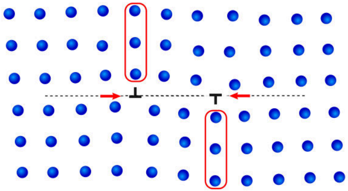
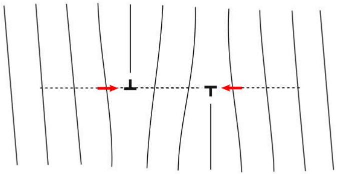
- Interactions between dislocations





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)
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  - • hexagonal close packed (hcp)
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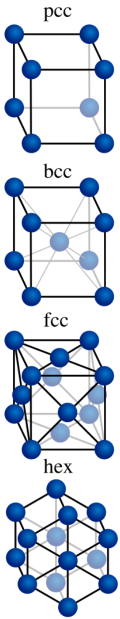
  + and 10 other bravais lattices.
- Slip planes $\boldsymbol{n} = (ijk)$ (often the most densely packed)
- slip systems $\boldsymbol{d} = [prs]$ (often the most densely packed)
  $(\boldsymbol{n} \cdot \boldsymbol{d} = ip + jr + ks = 0)$



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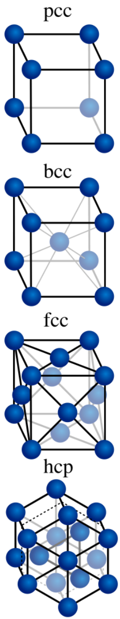

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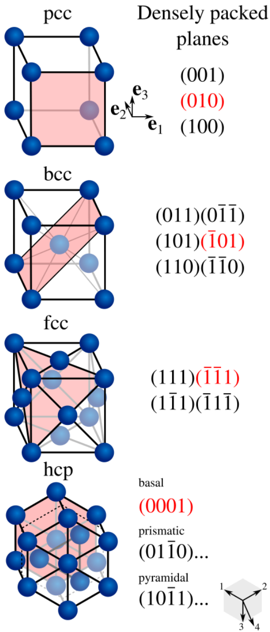

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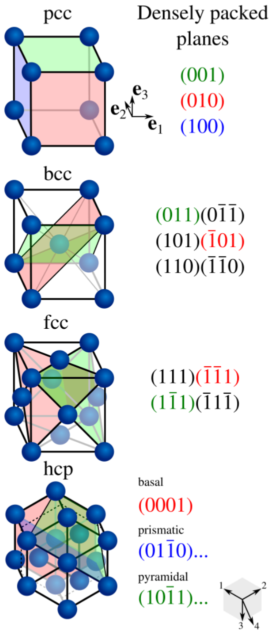

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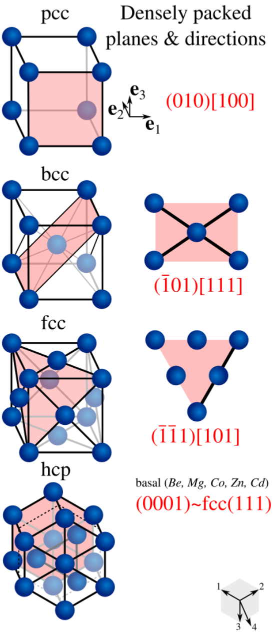

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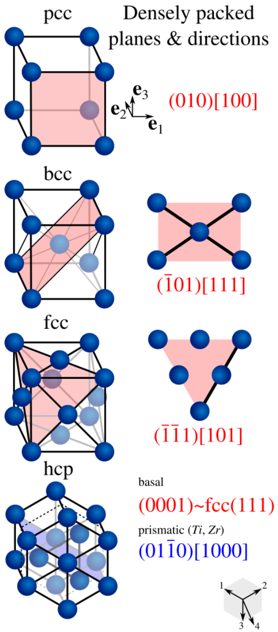
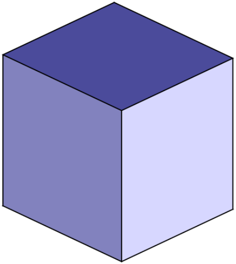


3D dislocations

- Slip plane $\boldsymbol{n}$
- Oriented dislocation line $\boldsymbol{\xi}$
- Burgers vector $\boldsymbol{b}$
  can be expressed in terms of minimal distance between atoms in the slip system
- Dislocation types:
  - edge *(coin)*: $\boldsymbol{b} \cdot \boldsymbol{\xi} = 0$
  - screw *(vis)*: $\boldsymbol{b} \times \boldsymbol{\xi} = 0, \quad \forall \boldsymbol{n}$
  - 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

3D dislocations

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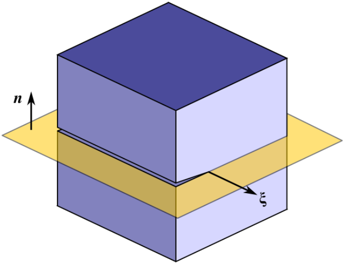

Introduce a cut along a densely packed plane with normal $\boldsymbol{n}$ (e.g. (111) in fcc)

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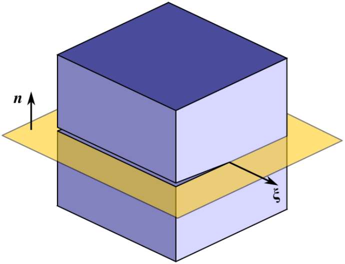

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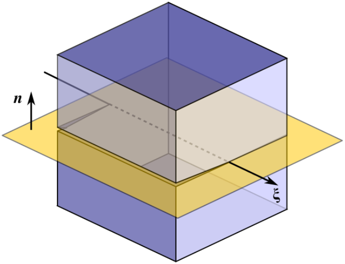

Cut's edge is the dislocation line, introduce an orientation $\boldsymbol{\xi}$

3D dislocations

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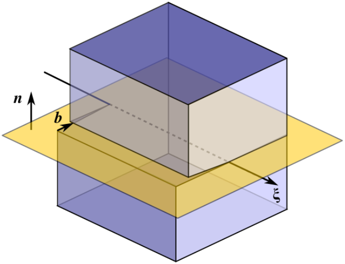

Shift the cut by a vector $\boldsymbol{b}$ along the plane **orthogonally** to the dislocation line and glue sides
Edge dislocation

3D dislocations

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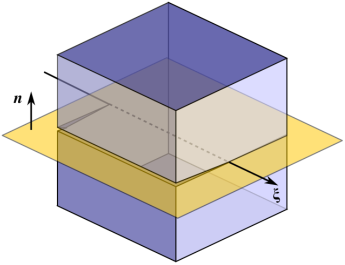

Cut in the box

3D dislocations

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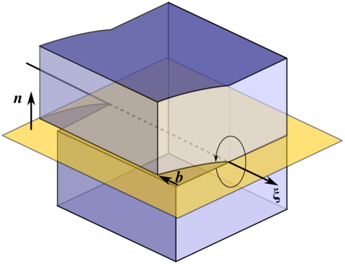

Shift the cut by a vector $\boldsymbol{b}$ along the plane **parallel** to the dislocation line and glue sides
Screw dislocation

3D dislocations

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- Burgers vector $\boldsymbol{b}$
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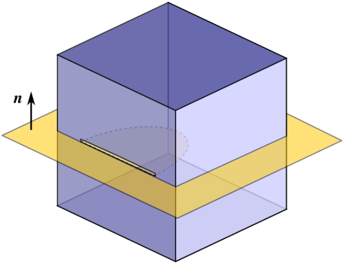

Semi-circular cut in the box

3D dislocations

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  - mixed
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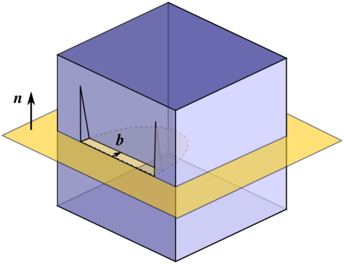

Shift the cut by a vector $\boldsymbol{b}$ and obtain a complex dislocation combining **screw and edge** dislocations

3D dislocations

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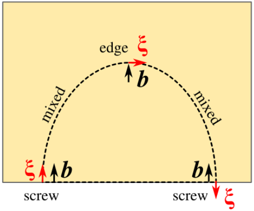

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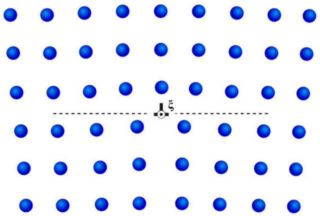

Edge dislocation

3D dislocations

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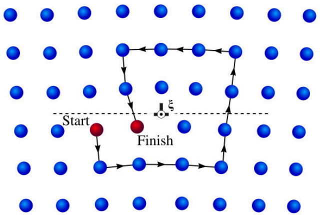

1 down, 3 right, 3 up, 3 left, 2 down

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

3D dislocations

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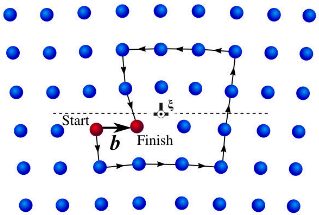

1 down, 3 right, 3 up, 3 left, 2 down

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

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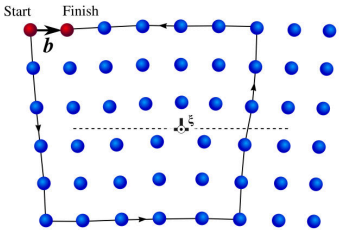

5 down, 5 right, 5 up, 5 left

Change the contour

3D dislocations

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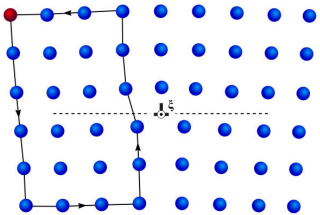

5 down, 3 right, 5 up, 3 left

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

3D dislocations

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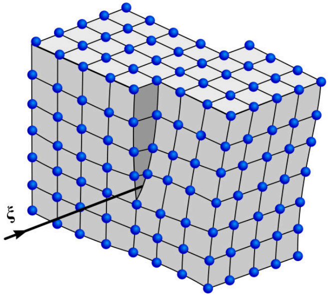

Screw dislocation

3D dislocations

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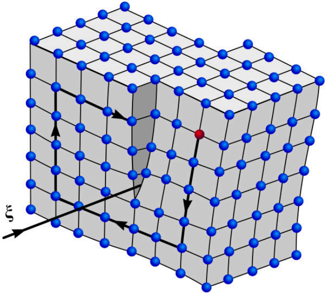

Draw a contour:
4 down, 5 left, 4 up, 3 right

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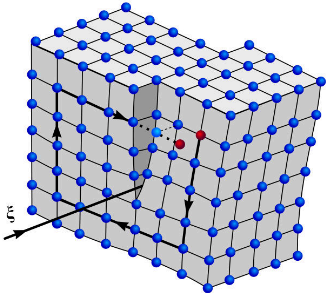

Draw a contour:
4 down, 5 left, 4 up, 3+2 right

3D dislocations

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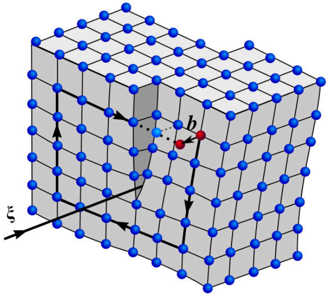
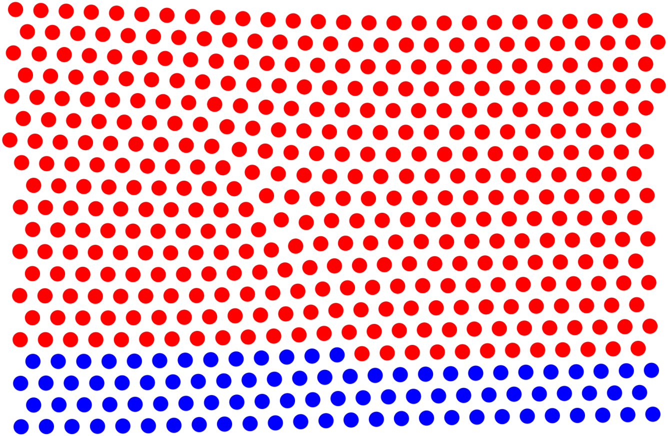


The Burgers vector is collinear with the dislocation line
$\boldsymbol{b} \parallel \xi$

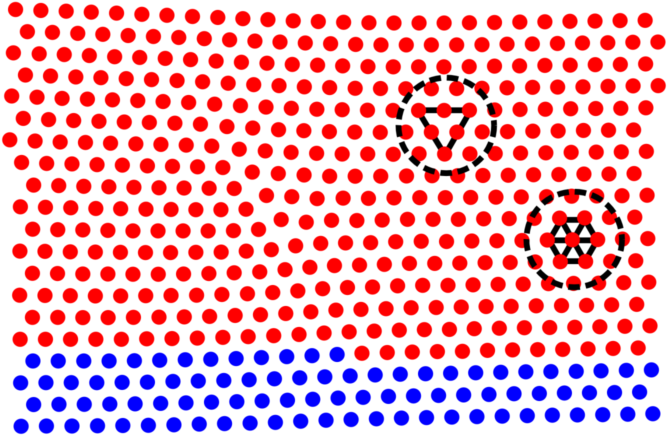
Burgers curcuit example

Example from the Monday lecture on Molecular dynamics



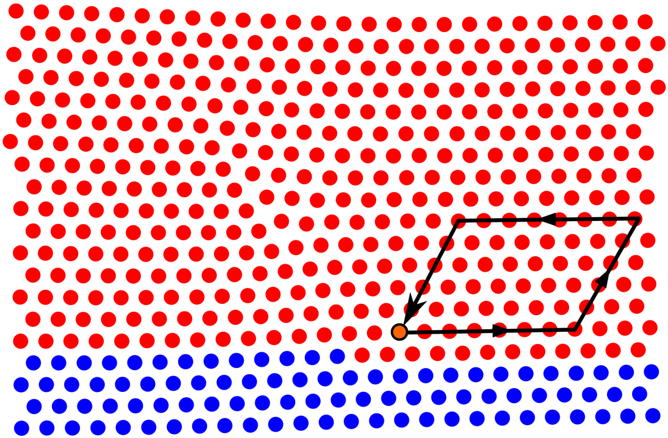
Burgers curcuit example

Example from the Monday lecture on Molecular dynamics



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

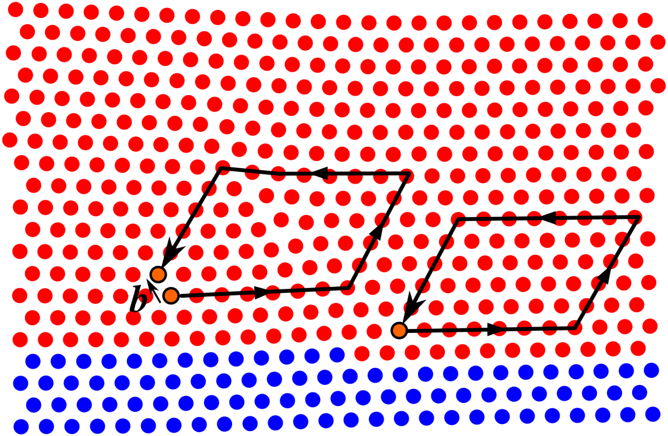
Example from the Monday lecture on Molecular dynamics



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

Burgers curcuit example

Example from the Monday lecture on Molecular dynamics



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

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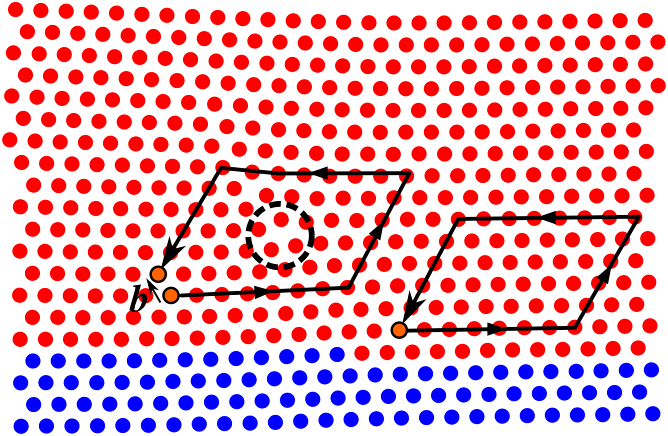

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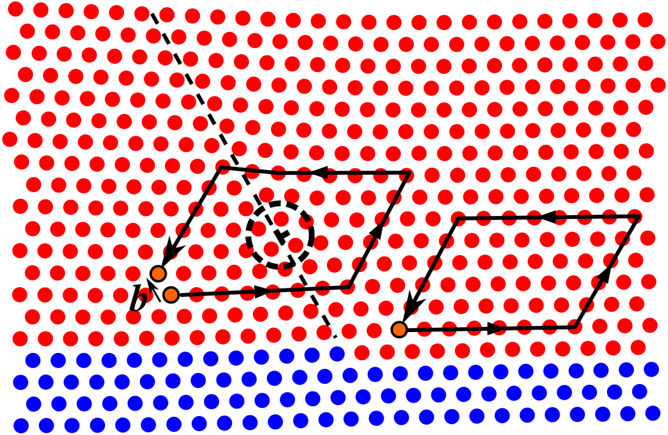


Contour 2: $\boldsymbol{b} = \frac{a}{\sqrt{2}}[\bar{1}10]$

Forces on dislocations

- A uniform stress σ shears a single crystal
- Force on the top $f = \int \sigma \cdot n dA = \sigma_n wl$
- Work of this force on shearing the crystal by amount $b = e_1|b|$:

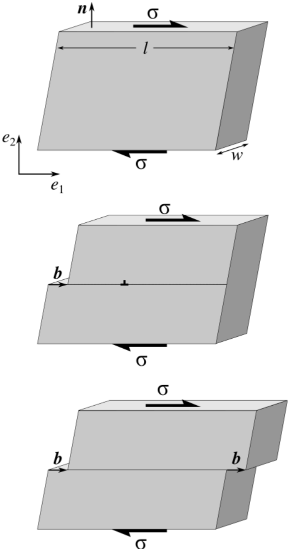
  $W = f \cdot b = wl\sigma_n \cdot b$
- At the same time dislocation of length w moves the distance l
- The "virtual" force f acting on the dislocation makes the same work:

  $wlf e_1 = W = wl\sigma_n \cdot b$ so

  $$f = (\sigma_n \cdot b)e_1$$
- More generally (valid for edge and screw dislocations)

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

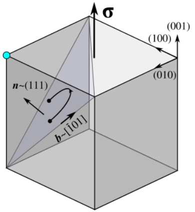
(Peach-Koehler force)



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

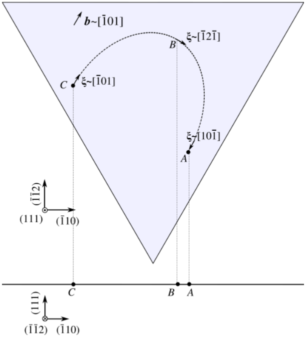
$$\boldsymbol{f} = (\boldsymbol{\sigma} \cdot \boldsymbol{b}) \times \boldsymbol{\xi}$$



- 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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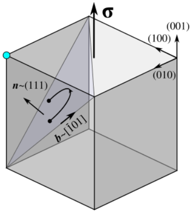

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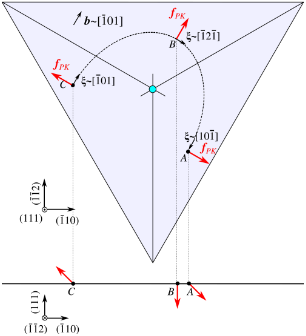

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Forces on dislocations

- 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

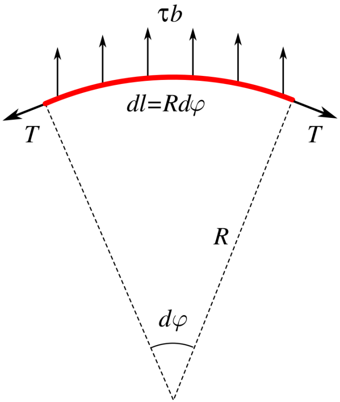
$$\boxed{T = \alpha\mu b^2}$$

- Then for a curved dislocation of radius R:

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

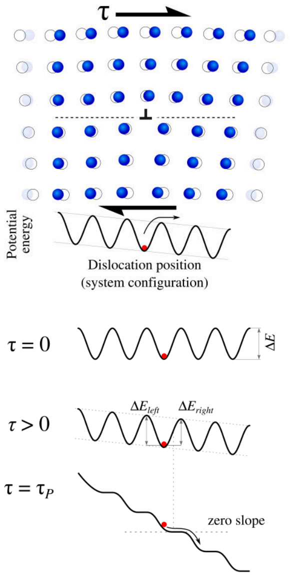
- For equilibrium (to keep this dislocation curved)

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



Dislocation motion

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



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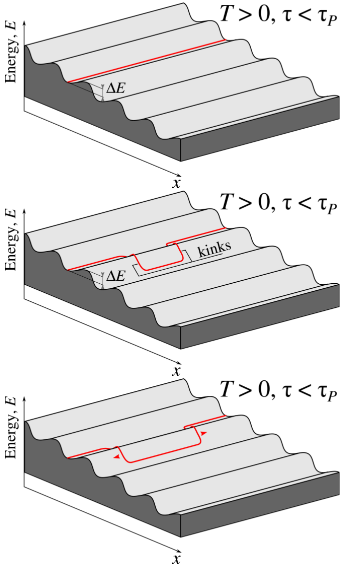
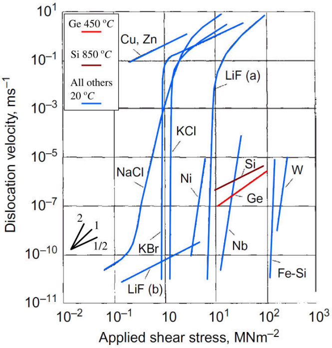


Dislocation motion

- 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

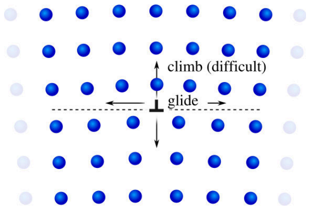
$$v_{\text{dis}} \sim f_{PK}, \quad f_{fr} \sim -g(T)v_{\text{dis}}$$

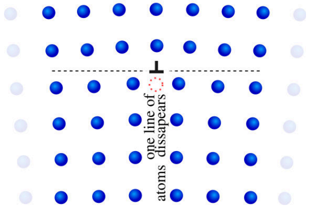
- Friction force f_{fr} comes from thermal vibrations of the lattice (phonons)
- In FCC: often viscous drag regime
- In BCC: viscous drag for edge and kinks-mechanism for screw



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 $\boldsymbol{f}_{PK} \cdot \boldsymbol{n} \neq 0$
- 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 $\boldsymbol{b} \parallel \boldsymbol{\xi}$
- Change of plane by screw dislocations results in **cross-slip**





Climb of screw dislocations requires addition or removal of atoms

Dislocation motion II

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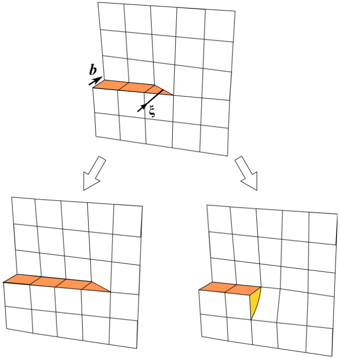

Screw dislocation may change the plane

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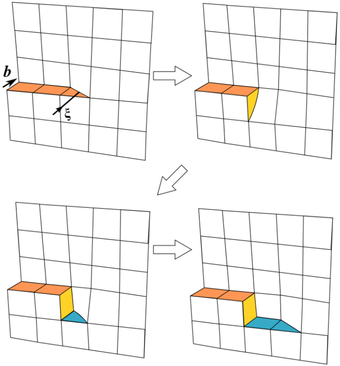
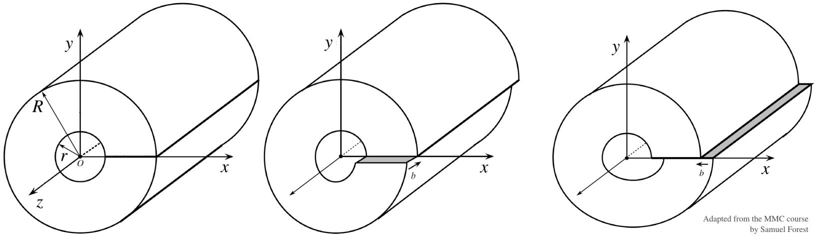


Cross-slip (imagine the remaining dislocation line)

- Volterra dislocation[1]



- Screw dislocation

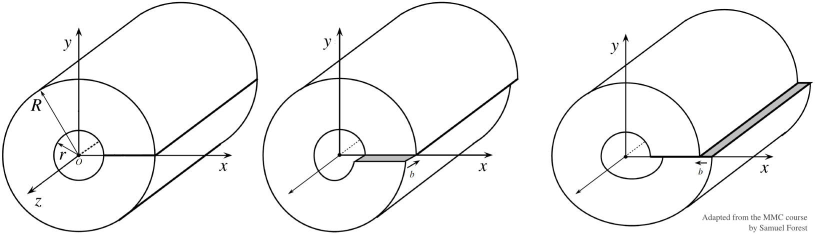
$$\sigma_{xz} = -\frac{\mu b}{2\pi}\frac{y}{(x^2+y^2)}$$
$$\sigma_{yz} = \frac{\mu b}{2\pi}\frac{x}{(x^2+y^2)}$$

- 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).

- Volterra dislocation[1]



- 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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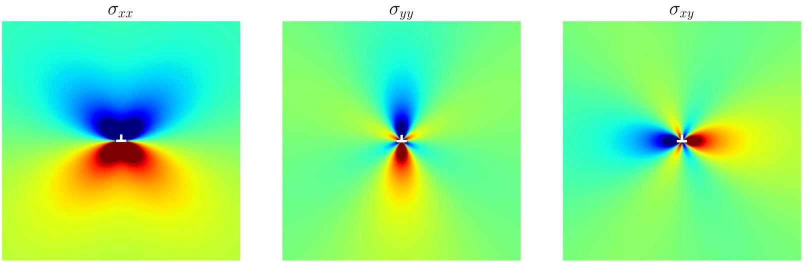
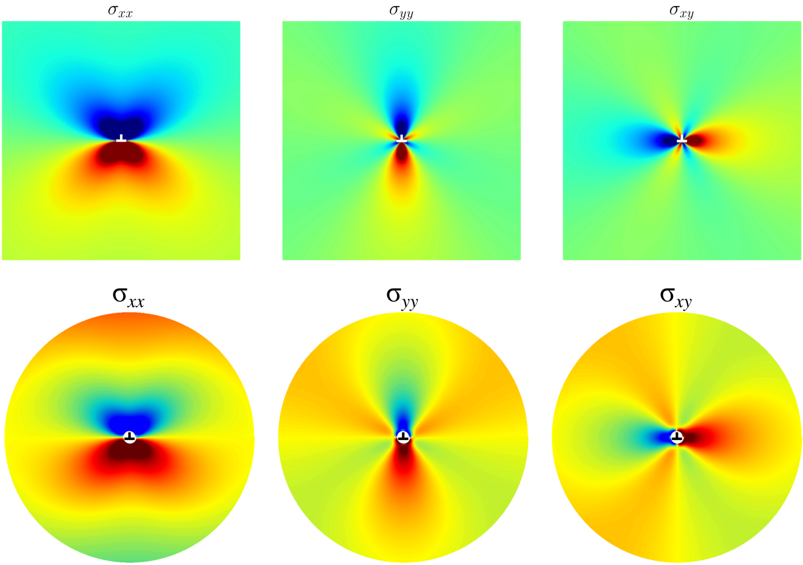
Dislocation-induced stress field



Theoretical stress field

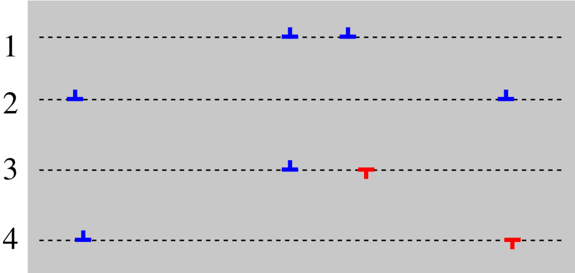
Dislocation-induced stress field



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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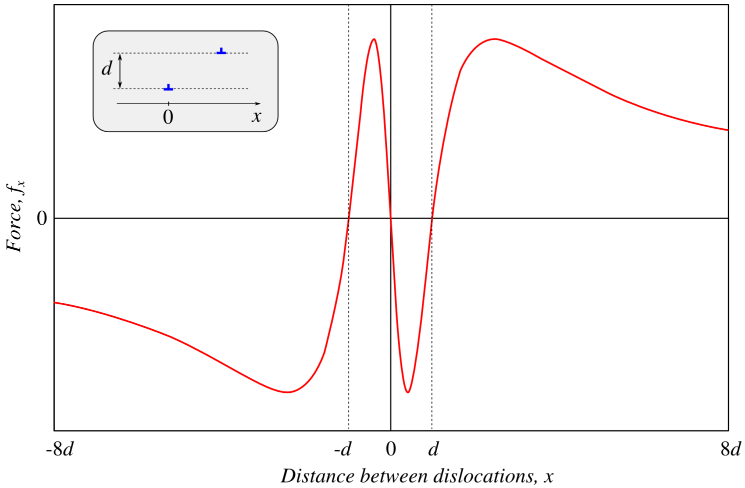

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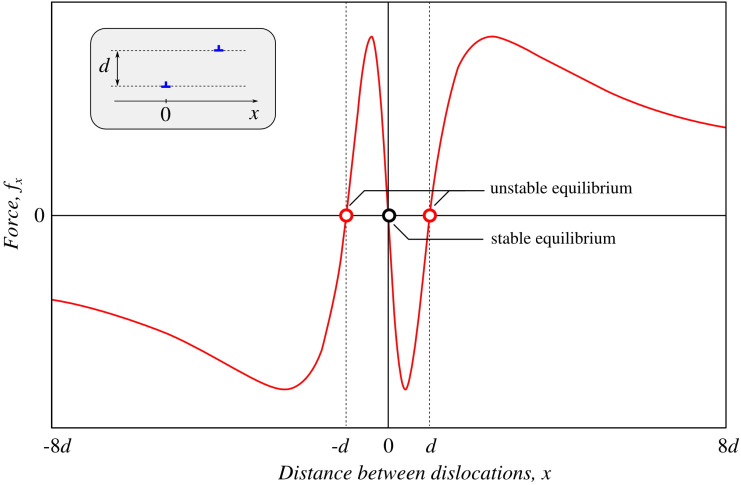

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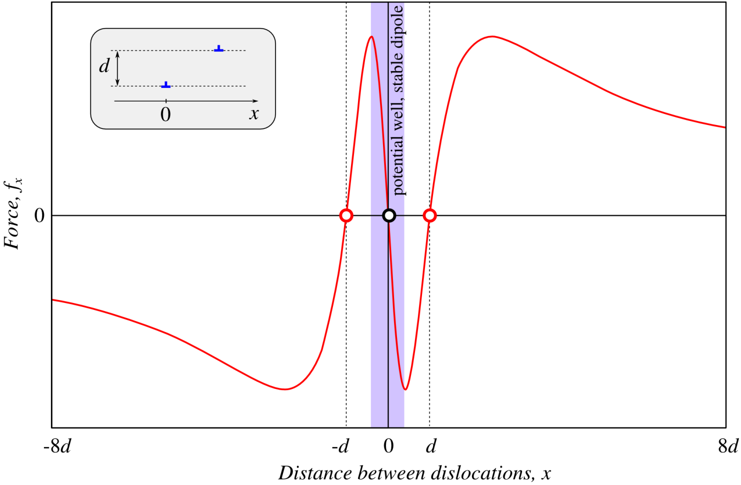

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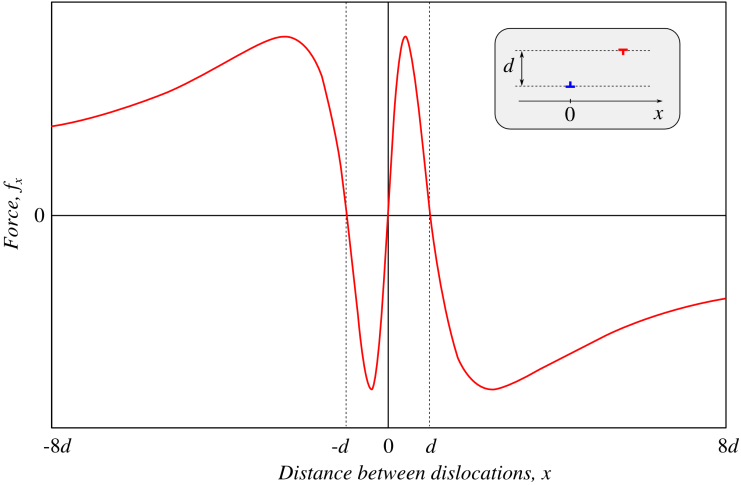

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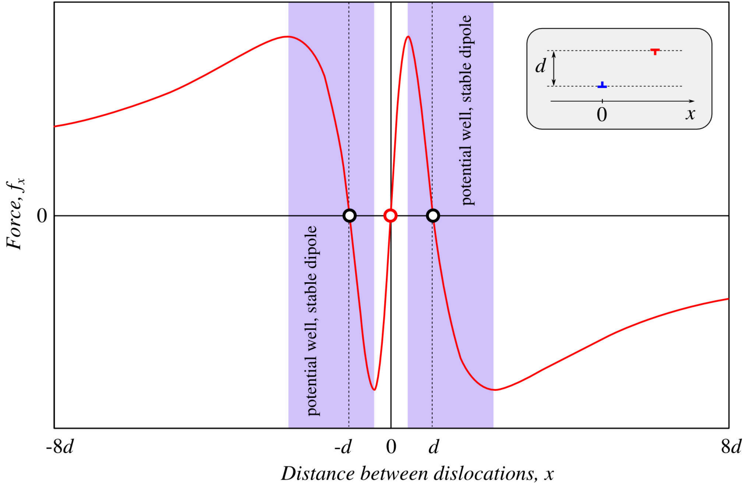

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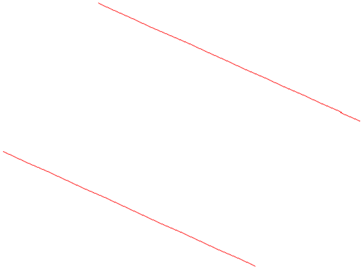

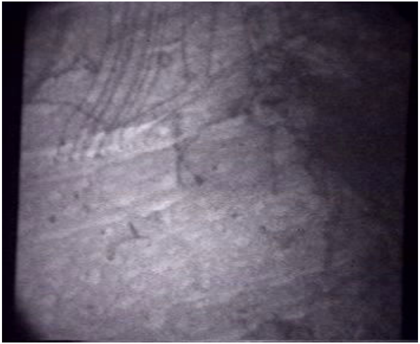

from Marc Fivel (SiMap, INP Grenoble), `www.numodis.fr/tridis`

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:

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

- 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

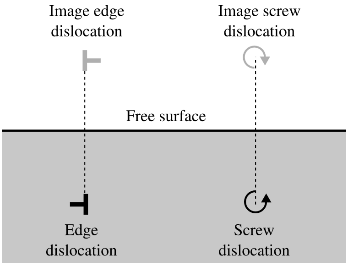

Image dislocation in air :)

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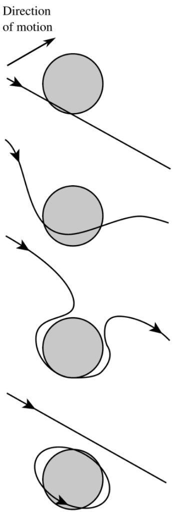

Interaction with a particle in dispersion-strengthened alloy
Orowan mechanism
Hirsch P.B., Humphreys F.J. Physics of Strength and Plasticity, Ed. A.S. Argon, MIT Press (1969)

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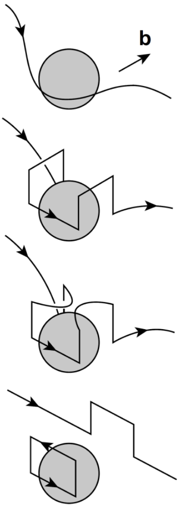

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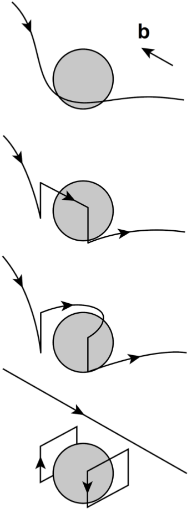

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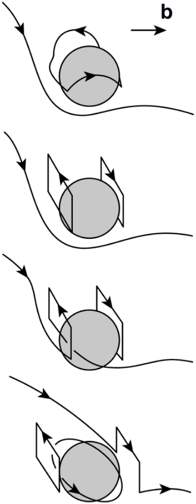

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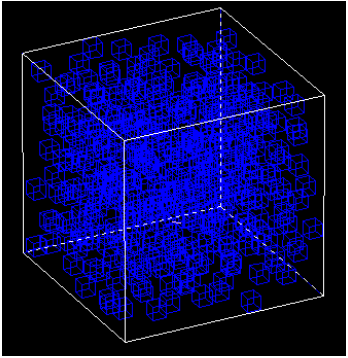

from Marc Fivel (SiMap, INP Grenoble),
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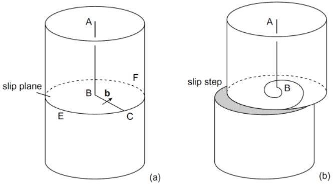
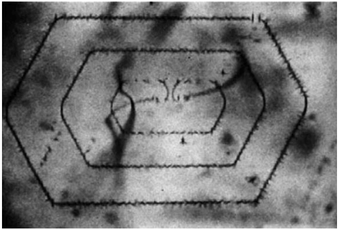
Origin of dislocations

- 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)

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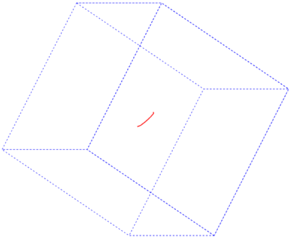
- In virgin well-annealed crystal
  $\rho \approx 10^{10}$ m^{-2}
- At early stages of deformation: single set of parallel slip planes is active
- At large deformation: $\rho \approx 10^{15}$ m^{-2}, different slip systems are activated
- At lattice defects and due to stress concentrators
- At grain 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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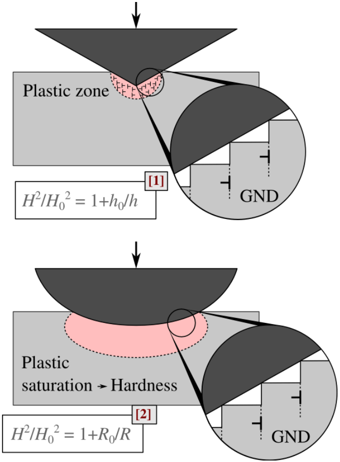


Size effect in nano-indentation due to geometrically necessary dislocations

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

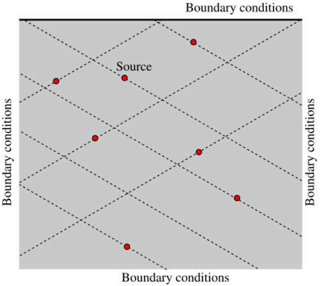
Simulation of dislocations in 2D

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)

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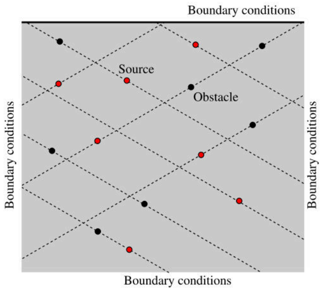

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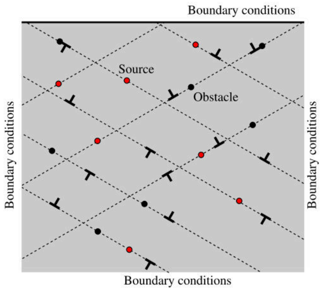

R. Van der Giessen, A. Needleman. Discrete dislocation plasticity: a simple planar model. Model Sim Mater Sci Eng (1995)

Simulation of dislocations in 2D

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 $|\boldsymbol{f}_i^{ext} + \boldsymbol{f}_i^d| \ge f_{nuc}$: 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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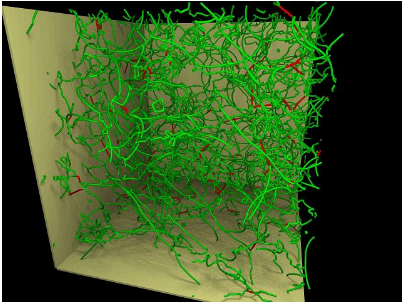
3D DD[1]

- 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*:

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

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

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)
- Bulatov V.V., Cai W. Computer Simulations of Dislocations, Oxford University Press, 2006.
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Merci de votre attention !