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Defects modeling in solid-state physics: coupling atomic scale with elasticity

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Robert Hooke (1635 – 1703)

ceiiinosssttuv

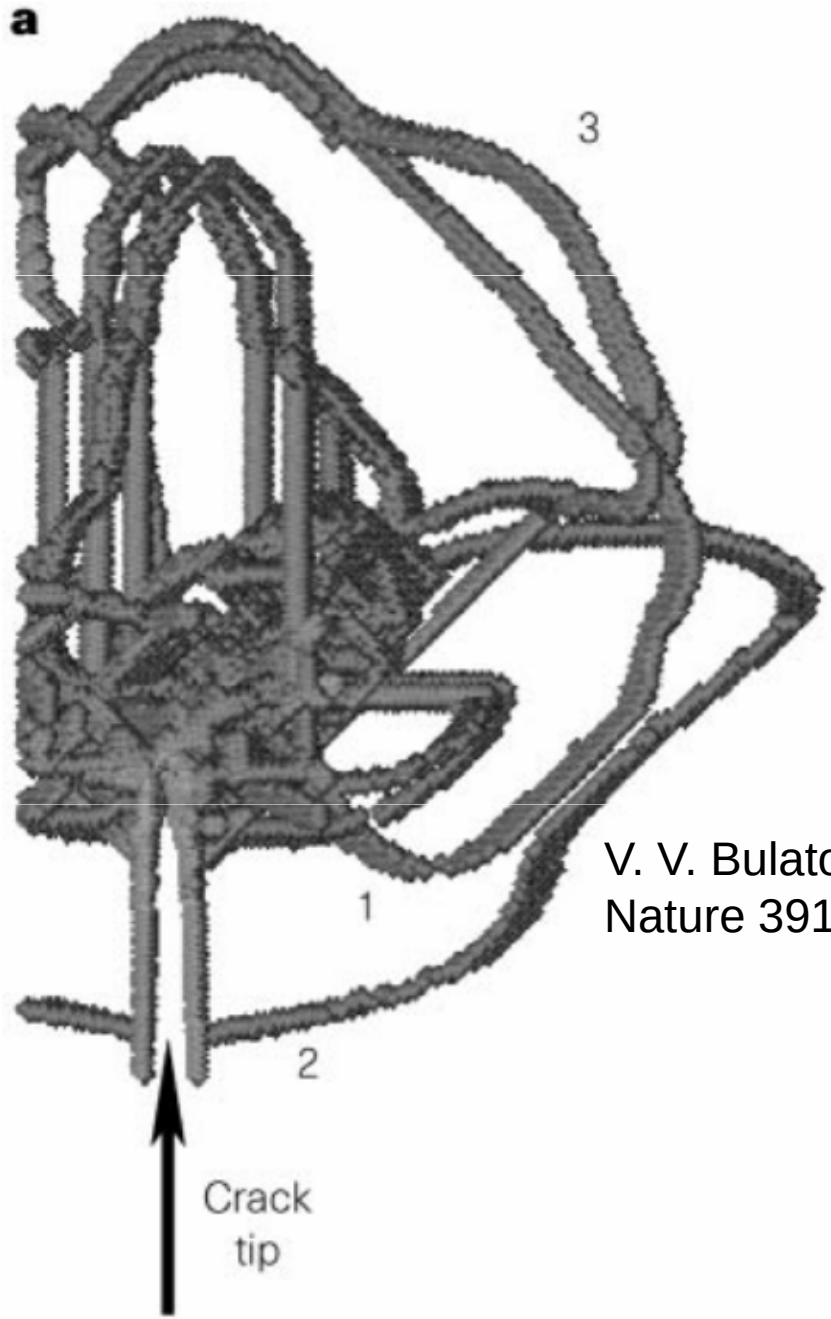
1660

Ut tensio, sic vis

As the extension, so the force

1678

source: wikipedia



Years 2000

Atomistic simulations
with several million atoms

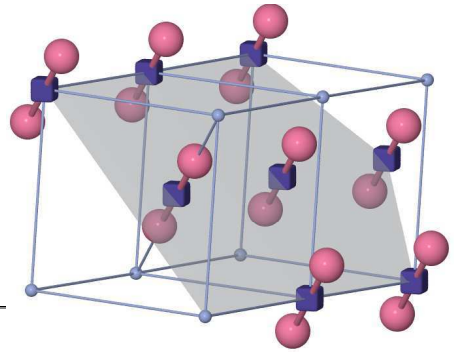
Molecular-dynamics simulations
of dynamic crack propagation
in a fcc crystal using 100 million atoms
with a Lennard-Jones potential

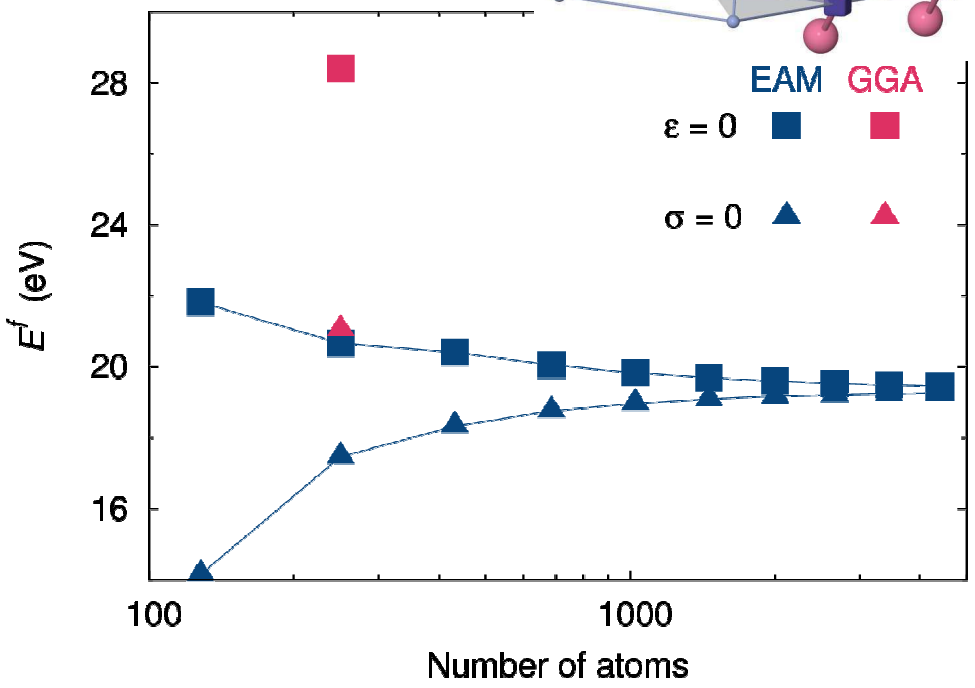
V. V. Bulatov, F. F. Abraham, L. P. Kubin, B. Devincre and S. Yip, Nature 391, 669 (1998).

Empirical potentials usually perfectly match elastic behaviour

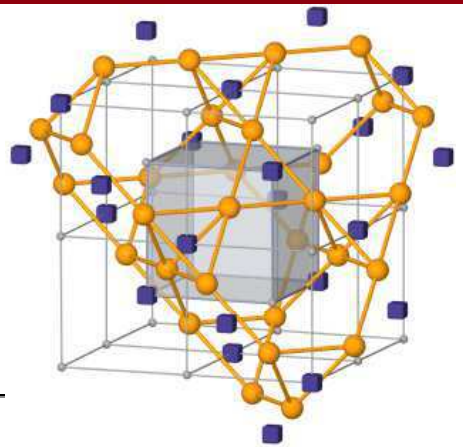
Self-interstitial clusters in bcc iron : Cluster containing 8 SIAs

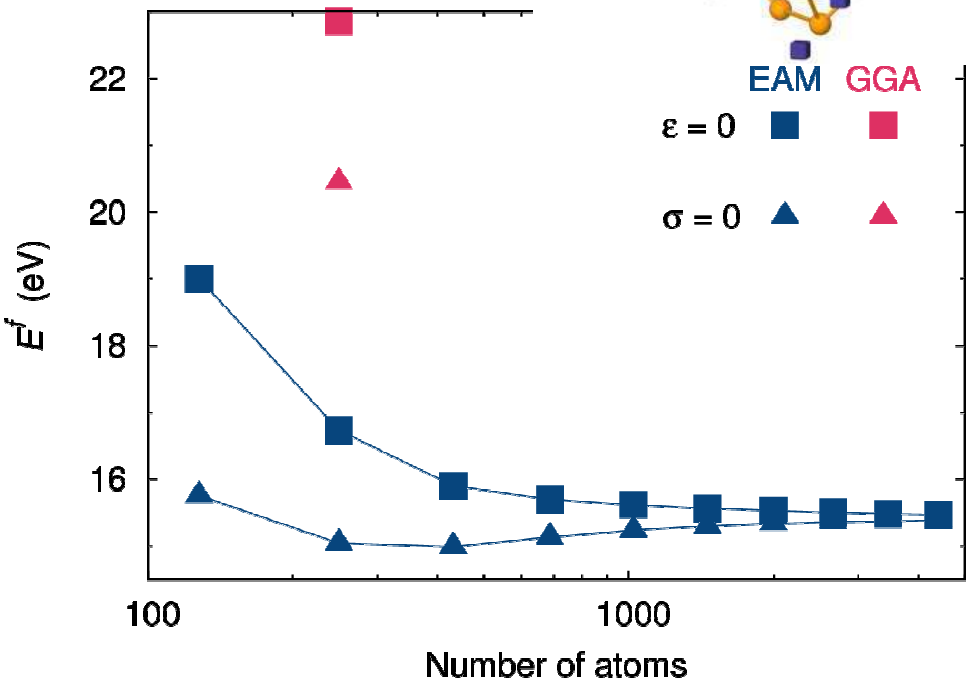
‹111› loop





C15 aggregate[1]





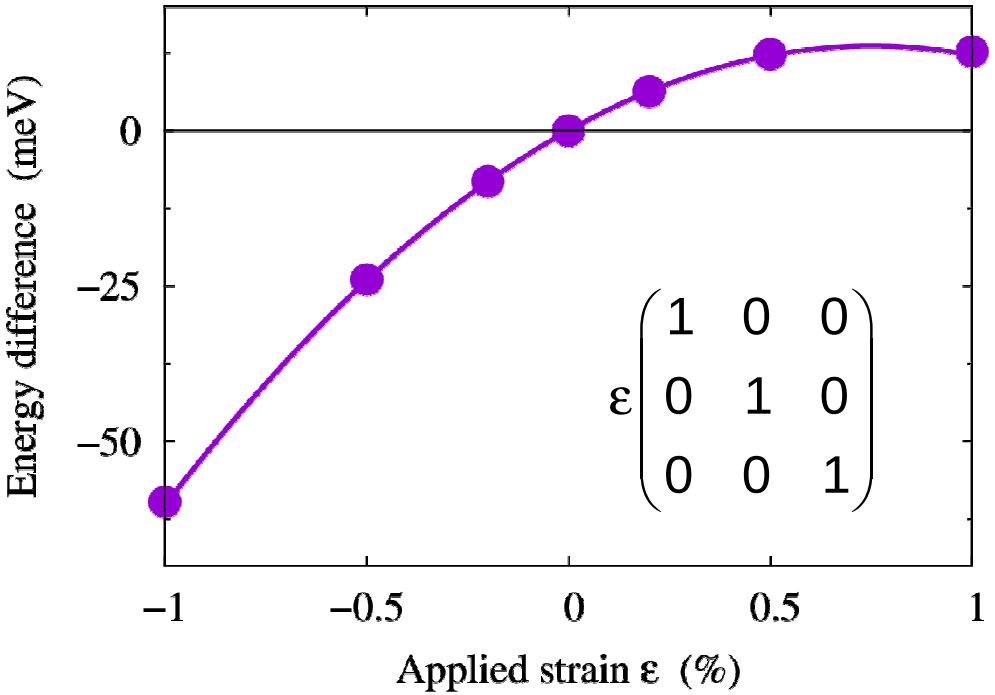
GGA ε=0 : ΔE = 5.6 eV
σ=0 : ΔE = 0.6 eV

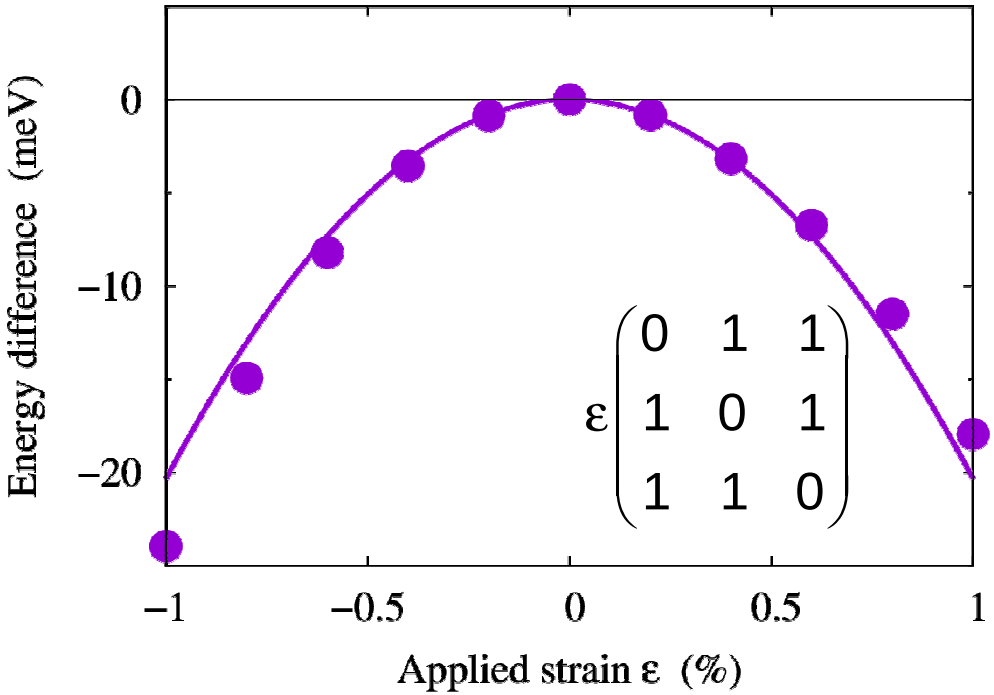
➔ elasticity can be used to understand (and withdraw) size effects in atomistic simulations

1 M.-C. Marinica, F. Willaime, and J.-P. Crocombette, Phys. Rev. Lett. **108**, 025501 (2012).

Vacancy in bcc iron : interaction with an applied strain

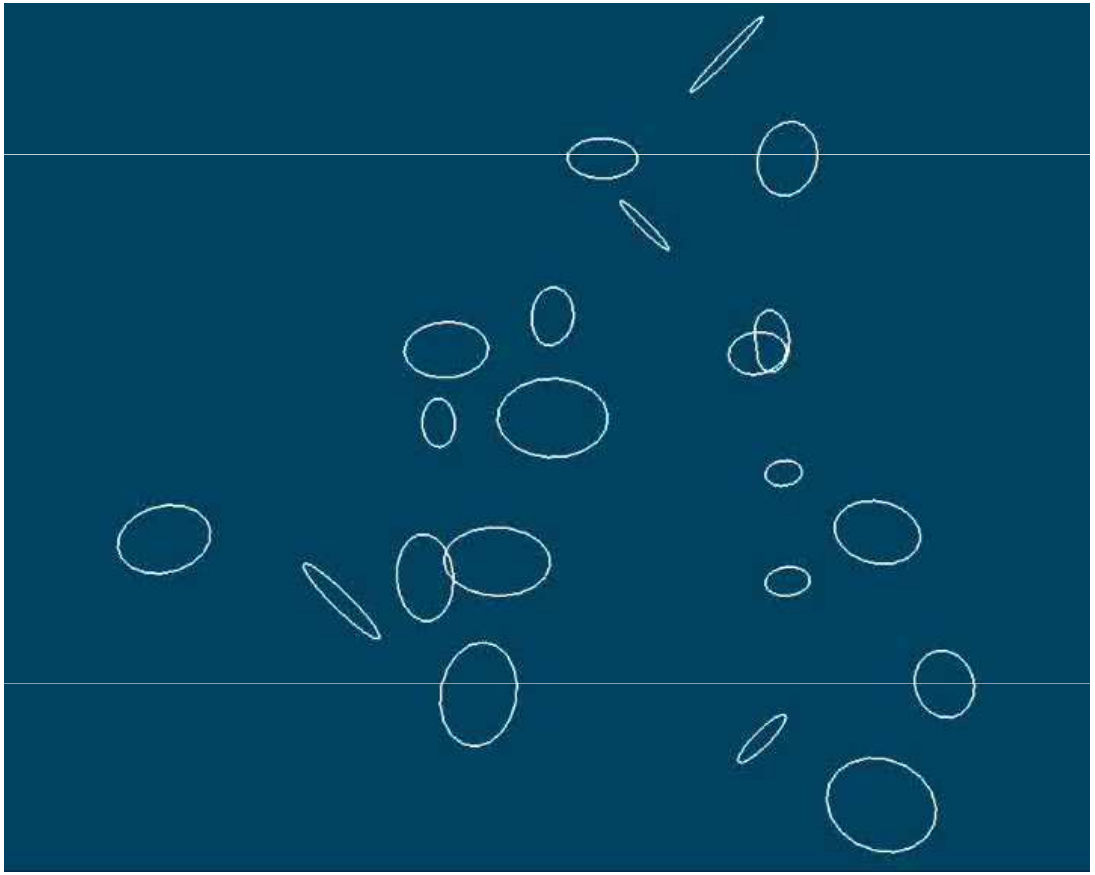
Simulation box 10x10x10 (2000 sites)
Marinica 2007 EAM potential





➔ elasticity can be used to model **variations with the applied strain** of the energies of defects (vacancies, self interstitials, solute, precipitates)

Dislocation dynamics simulations



Coarsening kinetics
of a distribution
of prismatic loops

2 time steps
- dislocation glide
- dislocation climb (diffusion)

Al parameters
T = 600K
unfaulted {110} loops

➔ elasticity can be used to model **microstructure evolution** at a mesoscopic scale (DD, phase field)

D. Mordehai, E. Clouet, M. Fivel, and M. Verdier, Philos. Mag. **88**, 899 (2008)
B. Bakó, E. Clouet, L. Dupuy and M. Blétry, Philos. Mag. **91**, 3173 (2011)

Outlines

I. Elasticity Theory

II. Inclusions, Inhomogeneities and Point Defects

III. Dislocations

IV. Plane interfaces

I . Elasticity Theory

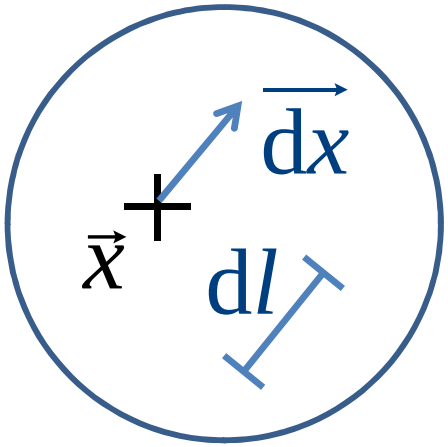
1. Deformation of an elastic body
2. Stresses in an elastic body
3. Thermodynamics of deformation
4. Hooke's law
5. Equilibrium equation in homogeneous elasticity

References:

- L. Landau & E. Lifchitz, *Theory of elasticity*, Course of theoretical physics, vol. 7 (1967)
- A. E. H. Love, *The mathematical theory of elasticity* (1927).
- J.P. Hirth & J. Lothe, *Theory of dislocations*, chap. 2 (1982)
- J. F. Nye, *Physical Properties of Crystals - Their representation by tensors and matrices* (1957).
- D. J. Bacon, D. M. Barnett and R. O. Scattergood, Prog. Mater. Sci. **23**, 51 (1980).

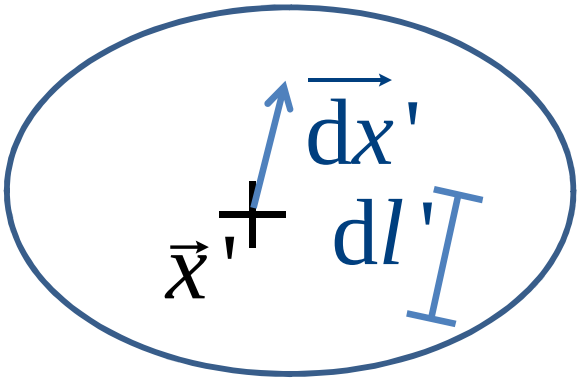
1. Deformation of an Elastic Body

Reference state



Deformation

Strained state



Displacement $\vec{u} = \vec{x}' - \vec{x}$: $u_i = x_i' - x_i$

Distortion $\mathbf{F} = \vec{\nabla} \otimes \vec{u}$: $F_{ij} = \partial u_i / \partial x_j$

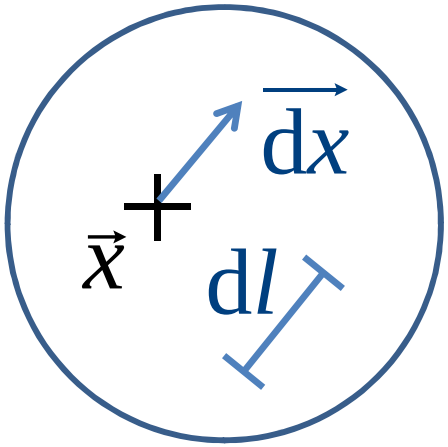
➔ $\mathrm{d}x_i' = \mathrm{d}x_i + \frac{\partial u_i}{\partial x_j}\mathrm{d}x_j = \left(\delta_{ij} + F_{ij}\right)\mathrm{d}x_j$

Strain $\boldsymbol{\varepsilon} = \frac{1}{2}\left[\left(\mathbf{Id}+\mathbf{F}\right)\left(\mathbf{Id}+\mathbf{F}^{\mathrm{t}}\right)-\mathbf{Id}\right]$: $\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\frac{\partial u_j}{\partial x_i}\right)$

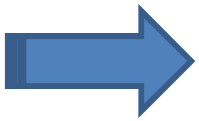
➔ $\mathrm{d}l'^2 = \mathrm{d}l^2 + 2\varepsilon_{ij}\mathrm{d}x_i\mathrm{d}x_j$

1. Deformation of an Elastic Body

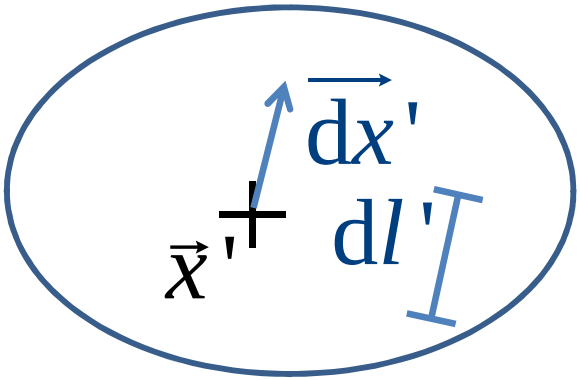
Reference state



Deformation



Strained state



Displacement $\vec{u} = \vec{x}' - \vec{x}$: $u_i = x_i' - x_i$

Distortion $\mathbf{F} = \vec{\nabla} \otimes \vec{u}$: $F_{ij} = \partial u_i / \partial x_j$

➔ $dx_i' = dx_i + \frac{\partial u_i}{\partial x_j} dx_j = \left(\delta_{ij} + F_{ij} \right) dx_j$

Strain $\boldsymbol{\varepsilon} = \frac{1}{2}\left[\left(\mathbf{Id} + \mathbf{F} \right)\left(\mathbf{Id} + \mathbf{F}^{\mathrm{t}} \right) - \mathbf{Id} \right]$ (Green-Lagrange)

$\boldsymbol{\varepsilon} = \frac{1}{2}\left[\mathbf{Id} - \left(\mathbf{Id} + \mathbf{F}^{\mathrm{t}} \right)^{-1} \left(\mathbf{Id} + \mathbf{F} \right)^{-1} \right]$ (Euler-Almansi)

symmetric 2nd rank tensors

Small deformation assumption

• Strain

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\mathbf{F} + \mathbf{F}^{\mathrm{t}}\right) : \varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

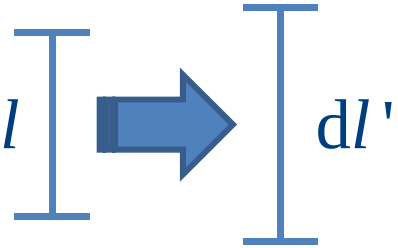
• Rotation

$$\boldsymbol{\Omega} = \frac{1}{2}\left(\mathbf{F} - \mathbf{F}^{\mathrm{t}}\right) : \Omega_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)$$

no contribution in linear elasticity because no internal torque

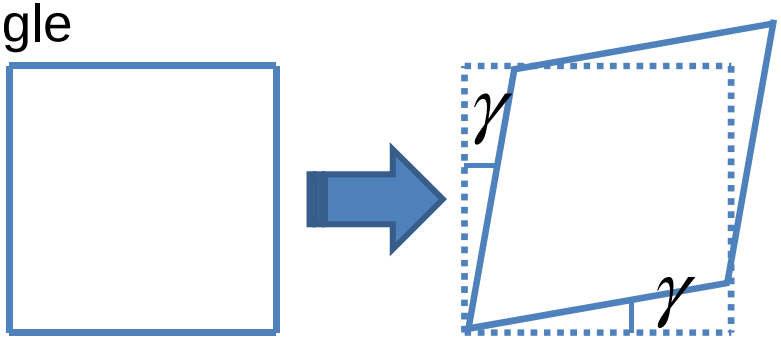
diagonal components:
elongation / compression

$$\varepsilon_{jj} = \frac{\mathrm{d}l' - \mathrm{d}l}{\mathrm{d}l}$$



off-diagonal components:
shear angle

$$\varepsilon_{ij} = \gamma$$



symmetric tensors

➔ 3 eigenvalues = elongation / compression along principal axes

volume change

$$\mathrm{d}V' = \mathrm{d}V(1+\varepsilon^{(1)})(1+\varepsilon^{(2)})(1+\varepsilon^{(3)})$$
$$= \mathrm{d}V(1+\varepsilon^{(1)}+\varepsilon^{(2)}+\varepsilon^{(3)})$$

➔ $\mathrm{Tr}(\boldsymbol{\varepsilon}) = \dfrac{\mathrm{d}V' - \mathrm{d}V}{\mathrm{d}V}$

1. Deformation of an Elastic Body

Small strain

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\vec{\nabla} \otimes \vec{u} + \vec{u} \otimes \vec{\nabla}\right) : \varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Spherical coordinates

$$\varepsilon_{rr} = \frac{\partial u_r}{\partial r}$$

$$\varepsilon_{\theta\theta} = \frac{u_r}{r} + \frac{1}{r}\frac{\partial u_\theta}{\partial \theta}$$

$$\varepsilon_{\phi\phi} = \frac{u_r}{r} + \frac{u_\theta}{r}\cot\theta + \frac{1}{r\sin\theta}\frac{\partial u_\phi}{\partial \phi}$$

$$2\varepsilon_{\theta\phi} = \frac{1}{r}\left(\frac{\partial u_\phi}{\partial \theta} - u_\phi \cot\theta\right) + \frac{1}{r\sin\theta}\frac{\partial u_\theta}{\partial \phi}$$

$$2\varepsilon_{r\phi} = \frac{\partial u_\phi}{\partial r} - \frac{u_\phi}{r} + \frac{1}{r\sin\theta}\frac{\partial u_r}{\partial \phi}$$

$$2\varepsilon_{r\theta} = \frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r} + \frac{1}{r}\frac{\partial u_r}{\partial \theta}$$

Cylindrical coordinates

$$\varepsilon_{rr} = \frac{\partial u_r}{\partial r}$$

$$\varepsilon_{\theta\theta} = \frac{u_r}{r} + \frac{1}{r}\frac{\partial u_\theta}{\partial \theta}$$

$$\varepsilon_{zz} = \frac{\partial u_z}{\partial z}$$

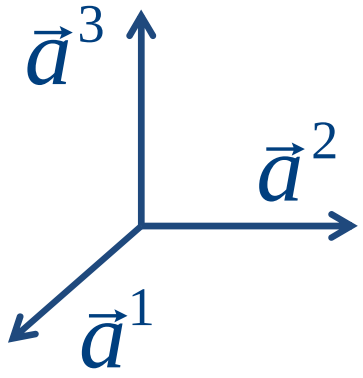
$$2\varepsilon_{\theta z} = \frac{\partial u_\theta}{\partial z} + \frac{1}{r}\frac{\partial u_z}{\partial \theta}$$

$$2\varepsilon_{rz} = \frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z}$$

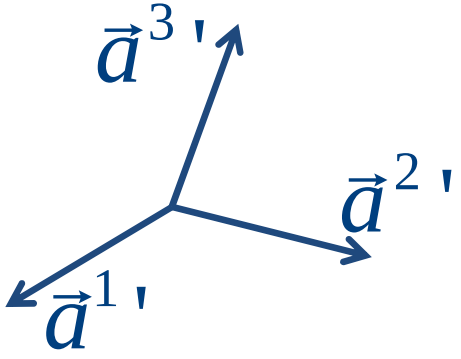
$$2\varepsilon_{r\theta} = \frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r} + \frac{1}{r}\frac{\partial u_r}{\partial \theta}$$

Strain extraction from atomistic simulations

- average strain: from vectors defining simulation cell (periodic or not)



Deformation



$$\mathbf{H} = \left(\vec{a}^1 \,|\, \vec{a}^2 \,|\, \vec{a}^3\right) \qquad \mathbf{H}' = \left(\vec{a}^1{}' \,|\, \vec{a}^2{}' \,|\, \vec{a}^3{}'\right)$$

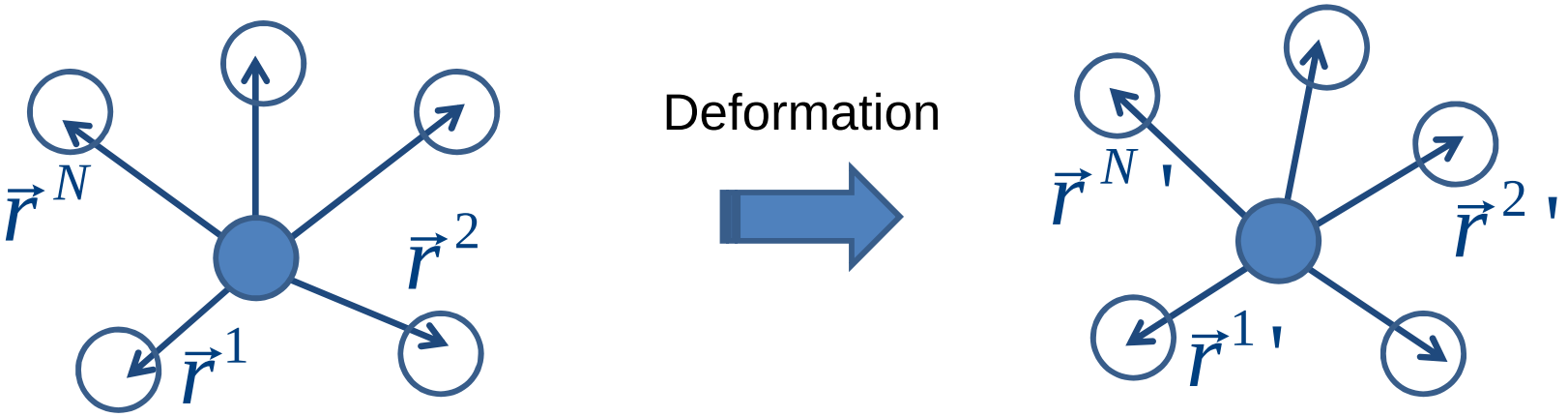
$$\mathbf{H}' = (\mathbf{Id} + \mathbf{F})\mathbf{H}$$

➔ distortion: $\mathbf{F} = \mathbf{H}'\,\mathbf{H}^{-1} - \mathbf{Id}$

➔ strain, rotation, …

Strain extraction from atomistic simulations

- local strain (on each atom): from vectors defining neighbours positions



$$\mathbf{R} = \left(\vec{r}^{\,1} \,|\, \vec{r}^{\,2} \,|\cdots|\, \vec{r}^{\,N}\right) \qquad \mathbf{R}' = \left(\vec{r}^{\,1}\,' \,|\, \vec{r}^{\,2}\,' \,|\cdots|\, \vec{r}^{\,N}\,'\right)$$

$$\vec{r}^{\,n}\,' = (\mathbf{Id} + \mathbf{F})\vec{r}^{\,n},\ \forall n \in [\![1 : N]\!]$$

over-determined system: least square fitting

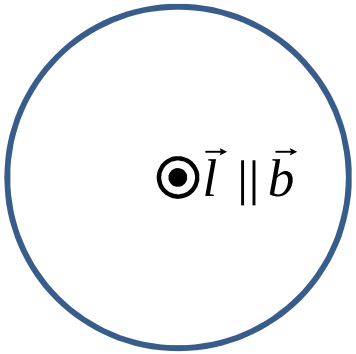
➔ distortion $\mathbf{F} = \left(\mathbf{R}'\,\mathbf{R}^t\right)\left(\mathbf{R}\,\mathbf{R}^t\right)^{-1} - \mathbf{Id}$

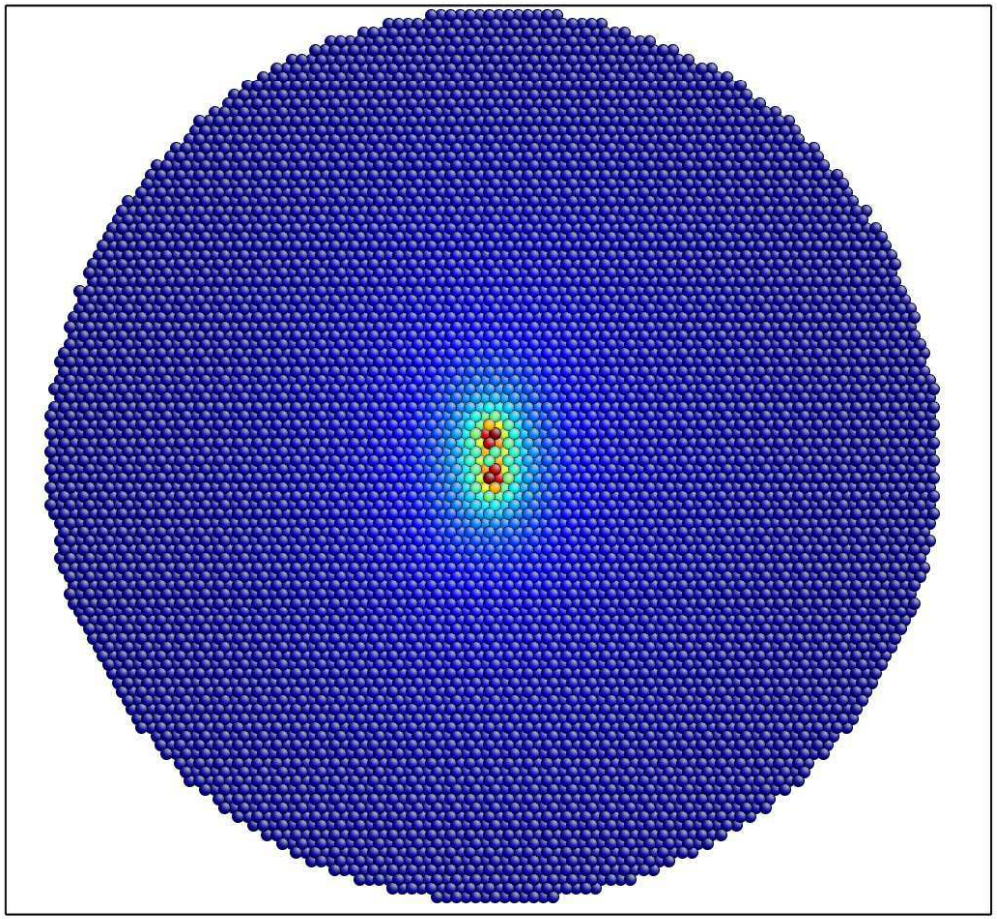
➔ strain, rotation, …

C. S. Hartley and Y. Mishin, Acta Mater. **53**, 1313 (2005).

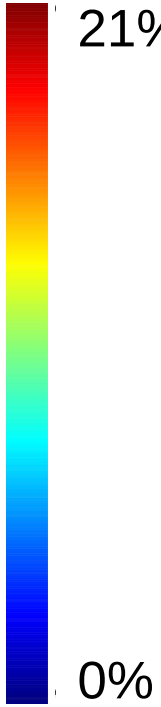
Strain extraction from atomistic simulations

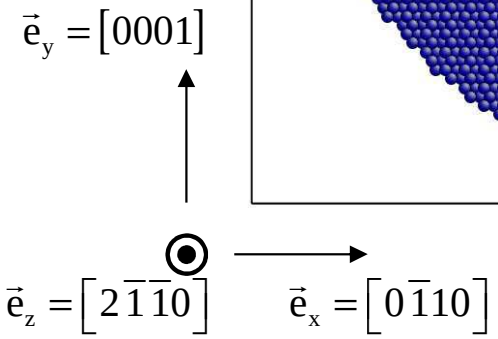
screw dislocation in hcp Zr (EAM)





Trace of the deviatoric strain tensor
~ average shear





Visualization: atomeye (Ju Li, MIT)

J. Li, Modelling Simul. Mater. Sci. Eng. **11**, 173 (2003).

Force acting on a volume element of a **strained** body $\int_V \vec{F}\,\mathrm{d}V$

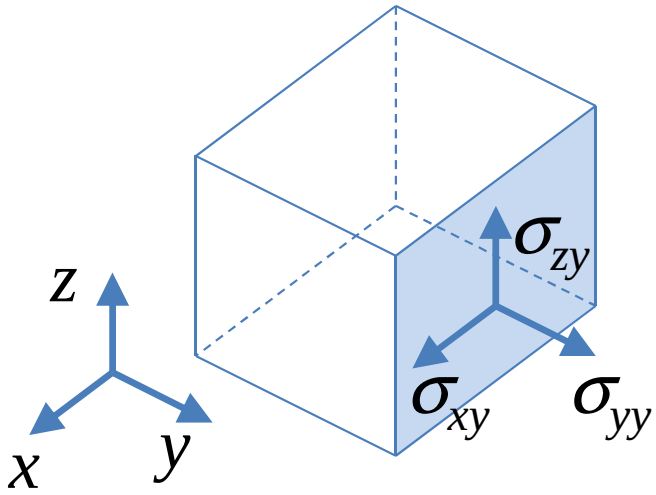
- external body force (gravity, distribution of point forces, …)

$$\vec{f}\,\mathrm{d}V$$

- internal forces corresponding to interaction between particles
  - cancellation of forces between particles inside V (action – reaction)
  - only forces corresponding to interaction with outside particles
    - ➔ proportional to the surface (no long range interaction)

$$\boldsymbol{\sigma}\,\overrightarrow{\mathrm{d}S}$$

$$\int_V F_i\,\mathrm{d}V = \int_V f_i\,\mathrm{d}V + \oint_S \sigma_{ij}\,\mathrm{d}S_j$$



Example: pressure

$$\boldsymbol{\sigma} = -P\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Equilibrium: no resultant **inside**

Force
$$\int_V F_i \mathrm{d}V = \int_V f_i \mathrm{d}V + \oint_S \sigma_{ij} \mathrm{d}S_j$$
$$= \int_V \left(f_i + \frac{\partial \sigma_{ij}}{\partial x_j} \right) \mathrm{d}V$$

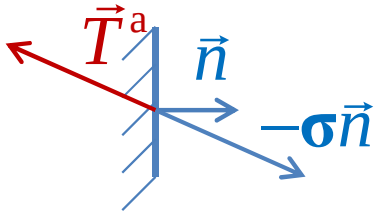
$$f_i + \frac{\partial \sigma_{ij}}{\partial x_j} = 0$$

Torque
$$\int_V M_{ik} \mathrm{d}V = \int_V \left(x_k f_i - x_i f_k \right) \mathrm{d}V + \oint_S \left(x_k \sigma_{ij} - x_i \sigma_{kj} \right) \mathrm{d}S_j$$
$$= \int_V \left(x_k f_i - x_i f_k \right) \mathrm{d}V + \int_V \frac{\partial}{\partial x_j} \left(x_k \sigma_{ij} - x_i \sigma_{kj} \right) \mathrm{d}V$$
$$= \int_V \left(\sigma_{ik} - \sigma_{ki} \right) \mathrm{d}V$$

$$\sigma_{ik} = \sigma_{ki}$$

+ equilibrium with applied forces
at the boundary

$$\vec{T}^{\mathrm{a}} \mathrm{d}S - \boldsymbol{\sigma} \overrightarrow{\mathrm{d}S} = \vec{0}$$



$$\sigma_{ij} n_j = T_j^{\mathrm{a}}$$

3. Thermodynamics of Deformation

Infinitesimal deformation corresponding to a displacement change $\delta\vec{u}$

Work of the internal forces

($\delta W > 0$ when energy flux from elastic body to outside)

$$\int_V \delta W \, \mathrm{d}V = -\int_V f_i \, \delta u_i \, \mathrm{d}V - \oint_S \sigma_{ij} \delta u_i \mathrm{d}S_j$$

$$= -\int_V f_i \, \delta u_i \, \mathrm{d}V - \int_V \frac{\partial}{\partial x_j}\left(\sigma_{ij} \delta u_i\right)\mathrm{d}V$$

$$= -\int_V \sigma_{ij} \frac{\partial \delta u_i}{\partial x_j}\mathrm{d}V$$

$$= -\int_V \sigma_{ij} \delta\varepsilon_{ij}\mathrm{d}V$$

Variation of the internal energy:
(defined per volume unit of the unstrained body)

$$\delta e = T\delta s - \delta w = T\delta s + \sigma_{ij}\delta\varepsilon_{ij}$$

of the free energy:

$$\delta f = \delta e - \delta(Ts) = s\delta T + \sigma_{ij}\delta\varepsilon_{ij}$$

➔

$$\sigma_{ij} = \left(\frac{\partial e}{\partial \varepsilon_{ij}}\right)_S = \frac{1}{V_0}\left(\frac{\partial E}{\partial \varepsilon_{ij}}\right)_S$$

$$\sigma_{ij} = \left(\frac{\partial f}{\partial \varepsilon_{ij}}\right)_T = \frac{1}{V_0}\left(\frac{\partial F}{\partial \varepsilon_{ij}}\right)_T$$

Example: hydrostatic strain

$$\delta\boldsymbol{\varepsilon} = \frac{\delta V}{3V_0}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\delta e = T\delta s + \sigma_{ij}\delta\varepsilon_{ij}$$

$$= T\delta s + \frac{\delta V}{3V_0}\sigma_{ij}\delta_{ij}$$

$$= T\delta s - P\frac{\delta V}{V_0} \qquad \text{with} \quad P = -\frac{1}{3}\mathrm{Tr}(\boldsymbol{\sigma})$$

$$\sigma_{ij} = \frac{1}{V_0}\frac{\partial E}{\partial\varepsilon_{ij}}\bigg|_S = \frac{1}{V_0}\frac{\partial F}{\partial\varepsilon_{ij}}\bigg|_T \quad \leftrightarrow\rightarrow \quad P = -\left(\frac{\partial E}{\partial V}\right)_S = -\left(\frac{\partial F}{\partial V}\right)_T$$

Constant pressure ensemble: $H = E + PV \quad \Rightarrow \quad \delta H = T\delta S + V\delta P$

Constant stress ensemble: $H = E - V_0\sigma_{ij}\varepsilon_{ij} \quad \Rightarrow \quad \delta H = T\delta S - V_0\varepsilon_{ij}\delta\sigma_{ij}$

Stress from atomistic simulations: average stress

N atoms in interaction $E = \sum_\alpha \frac{\vec{p}^\alpha \vec{p}^\alpha}{2m^\alpha} + E^{\text{int}}$ $\sigma_{ij} = -\frac{NkT}{V}\delta_{ij} + \frac{1}{V}\frac{\partial E^{\text{int}}}{\partial \varepsilon_{ij}}$

when the potential energy E^{int} only depends on atom positions $\vec{X}^\alpha$

$$\sigma_{ij} = -\frac{NkT}{V}\delta_{ij} + \frac{1}{V}\sum_\alpha \frac{\partial E^{\text{int}}}{\partial X_k^\alpha}\frac{\partial X_k^\alpha}{\partial \varepsilon_{ij}} = -\frac{NkT}{V}\delta_{ij} - \frac{1}{V}\sum_\alpha F_i^\alpha X_j^\alpha$$

! in PBC, E^{int} also depends on periodicity vectors

in quantum mechanics: $E^{int} = \langle \phi | H | \phi \rangle$

➔ stress from Hellmann-Feynman theorem: $\sigma_{ij} = \frac{1}{V}\left\langle \phi \left| \frac{\partial H}{\partial \varepsilon_{ij}} \right| \phi \right\rangle$

O. H. Nielsen and R. M. Martin, Phys. Rev. B **32**, 3780 (1985).

Stress from atomistic simulations: atomic stress

it cannot be always defined (not in ab initio)

one needs to be able - to partition the energy in atom contributions

- to associate a volume V^α to each atom

it has to be meaningful (average, equilibrium) $\boldsymbol{\sigma} = \frac{1}{V}\sum_\alpha V^\alpha \boldsymbol{\sigma}^\alpha$

➔ not always an easy task !

PRL 114, 258102 (2015) PHYSICAL REVIEW LETTERS week ending 26 JUNE 2015

Examining the Mechanical Equilibrium of Microscopic Stresses in Molecular Simulations

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LaCàN, Universitat Politècnica de Catalunya–BarcelonaTech, 08034 Barcelona, Spain
(Received 3 November 2014; published 23 June 2015)

The microscopic stress field provides a unique connection between atomistic simulations and mechanics at the nanoscale. However, its definition remains ambiguous. Rather than a mere theoretical preoccupation, we show that this fact acutely manifests itself in local stress calculations of defective graphene, lipid bilayers, and fibrous proteins. We find that popular definitions of the microscopic stress violate the continuum statements of mechanical equilibrium, and we propose an unambiguous and physically sound definition.

3. Thermodynamics of Deformation

Stress from atomistic simulations: atomic stress

it cannot be always defined (not in ab initio)

one needs to be able - to partition the energy in atom contributions

- to associate a volume V^α to each atom

it has to be meaningful (average, equilibrium) $\boldsymbol{\sigma} = \frac{1}{V}\sum_\alpha V^\alpha \boldsymbol{\sigma}^\alpha$

➔ not always an easy task !

Example: potentials depending only on the distance between atoms

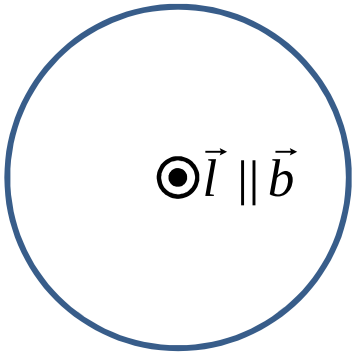
(pair potentials, EAM, 2nd moment approximation)

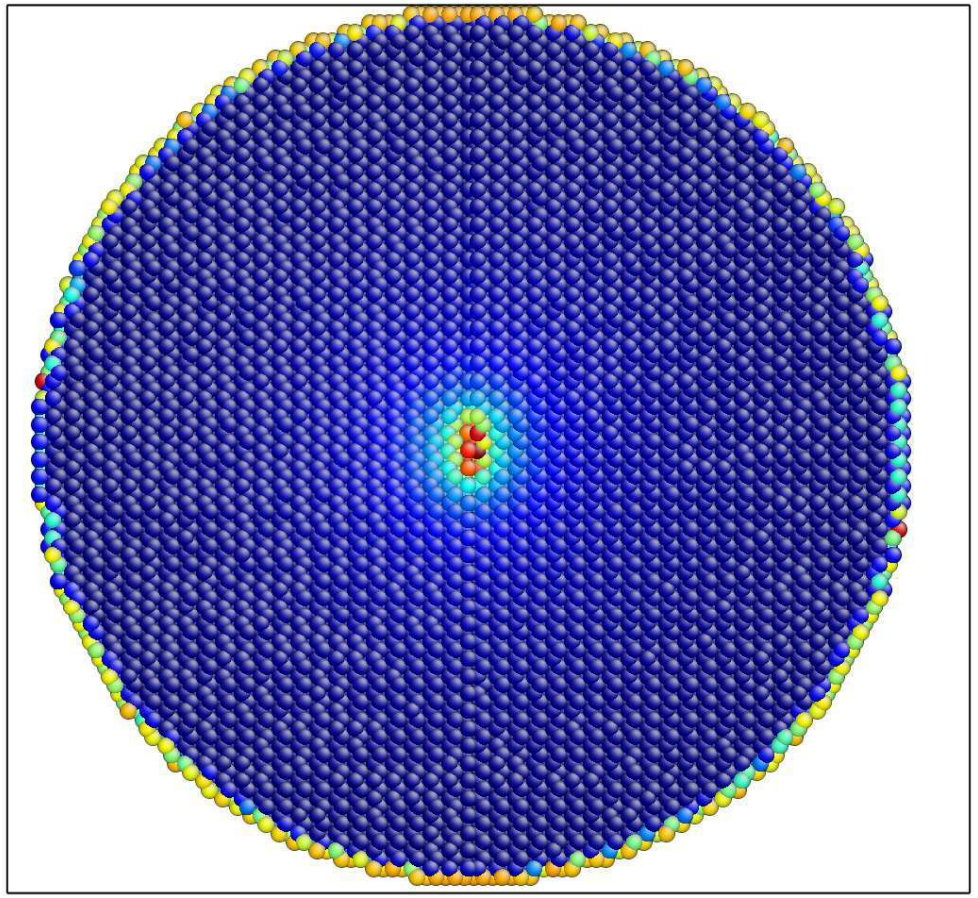
$$E^{\text{int}} = \phi\left(\left\{r_{\alpha\beta}\right\}\right) \qquad \sigma_{ij}^\alpha = \frac{1}{V^\alpha}\sum_\beta \frac{\partial\phi}{\partial r^{\alpha\beta}} \frac{\left(X_i^\alpha - X_i^\beta\right)\left(X_j^\alpha - X_j^\beta\right)}{\left(r^{\alpha\beta}\right)^2}$$

V. Vitek and T. Egami, Phys. Status Solidi B 144, 145 (1987).

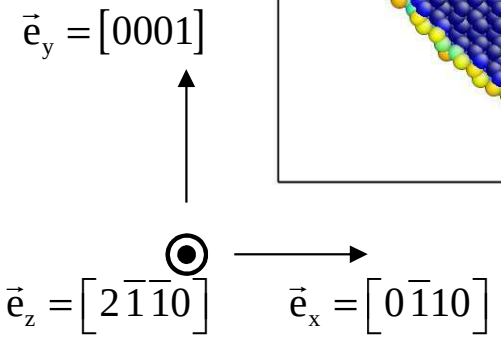
Stress from atomistic simulations: atomic stress

screw dislocation in hcp Zr (EAM)





Trace of the deviatoric stress tensor
= Von Misès stress



4. Hooke's Law

Thermodynamics: $\delta F = S\delta T + V\sigma_{ij}\delta\varepsilon_{ij}$ $\qquad \sigma_{ij} = \frac{1}{V}\left(\frac{\partial F}{\partial \varepsilon_{ij}}\right)_T$

➔ expression of $F(T,\boldsymbol{\varepsilon})$ needed

Undeformed state (reference):
elastic body at equilibrium without any external force (surface, body)

$$\sigma_{ij} = \frac{1}{V}\left(\frac{\partial F}{\partial \varepsilon_{ij}}\right)_T = 0$$

Small deformation assumption:

$$F(T,\boldsymbol{\varepsilon}) = F_0(T) + \frac{1}{2}VC_{ijkl}\varepsilon_{ij}\varepsilon_{kl}$$

➔ elastic constants: $C_{ijkl} = \frac{1}{V}\left(\frac{\partial^2 F}{\partial\varepsilon_{ij}\partial\varepsilon_{kl}}\right)_T$

➔ Hooke's law: $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$ ➔ $\Delta F = \frac{1}{2}V\sigma_{ij}\varepsilon_{ij}$

Hydrostatic strain $\varepsilon_{ij} = \frac{\Delta V}{3V}\delta_{ij}$ $\quad \sigma_{ij} = -P\delta_{ij}$ ➔ $P = -B\frac{\Delta V}{V}$ $\quad \Delta F = B\frac{\Delta V^2}{V}$

Properties of elastic constants

$$\Delta F = \frac{1}{2} V C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} > 0 \quad \forall \boldsymbol{\varepsilon}$$ ➔ C_{ijkl} : 4th rank tensor definite positive

$$\frac{\partial^2 F}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} = \frac{\partial^2 F}{\partial \varepsilon_{kl} \partial \varepsilon_{ij}}$$ ➔ $C_{ijkl} = C_{klij}$ (major symmetry)

$$\varepsilon_{ij} = \varepsilon_{ji}$$ ➔ $C_{ijkl} = C_{jikl} = C_{ijlk}$ (minor symmetries)

➔ **21 coefficients** (instead of 81)

Elastic compliance (inverse tensor)

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} \quad \rightarrow \quad \varepsilon_{ij} = S_{ijkl} \sigma_{kl} \quad \text{with} \quad C_{ijkl} S_{klmn} = \frac{1}{2} \left(\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm} \right)$$

4. Hooke's Law

Voigt notation

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \quad \rightarrow \quad \sigma_I = C_{IK}\varepsilon_K$$

sym. tensors in R^3 (6 components) → vectors in R^6 (6 components)

Indexes		Indexes
11		1
22		2
33		3
23 / 32	→	4
13 / 31		5
12 / 21		6

$$\Delta F = \frac{1}{2} V \sigma_{ij}\varepsilon_{ij} \quad \rightarrow \quad \Delta F = \frac{1}{2} V \sigma_I \varepsilon_I$$

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & & & & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{pmatrix}$$

$$\begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ & & S_{33} & S_{34} & S_{35} & S_{36} \\ & & & S_{44} & S_{45} & S_{46} \\ & & & & S_{55} & S_{56} \\ & & & & & S_{66} \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix}$$

$$C_{IK} = C_{ijkl} \quad \forall I, K$$

$$\begin{aligned} S_{IK} &= S_{ijkl} && \text{if } 1 \le I, K \le 3 \\ &= 2S_{ijkl} && \text{if } 1 \le I \le 3 \text{ and } 4 \le K \le 6 \\ &= 2S_{ijkl} && \text{if } 4 \le I \le 6 \text{ and } 1 \le K \le 3 \\ &= 4S_{ijkl} && \text{if } 4 \le I, K \le 6 \end{aligned}$$

Elastic constants and rotation

rotation $\mathbf{R}$: $\vec{u} \rightarrow \vec{u}' : \quad u'_i = R_{ij} u_j$

$$\mathbf{C} \rightarrow \mathbf{C}' : \quad C'_{ijkl} = R_{im} R_{jn} R_{ko} R_{lp} C_{mnop}$$

Elastic constants and symmetry

if $\mathbf{R}$ is a symmetry operation of the Bravais lattice

$$C_{ijkl} = R_{im} R_{jn} R_{ko} R_{lp} C_{mnop}$$

isotropic : 2 coefficients (Lamé coefficients)

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$$

cubic : 3 coefficients (C_{11}, C_{12}, C_{44})

hexagonal : 5 coefficients (C_{11}, C_{33}, C_{12}, C_{13}, C_{44})

4. Hooke's Law

Cubic elasticity

$$\begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ & C_{11} & C_{12} & 0 & 0 & 0 \\ & & C_{11} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & C_{44} \end{pmatrix} \qquad B = C_{11} + \frac{2}{3} C_{12}$$

Isotropic elasticity

$$C_{11} = \lambda + 2\mu \qquad C_{12} = \lambda \qquad C_{44} = \mu \qquad \rightarrow \qquad C_{44} = \frac{1}{2}(C_{11} - C_{12})$$

Bulk modulus: $B = \lambda + \frac{2}{3}\mu$

Young modulus: $E = \frac{\mu(3\lambda + 2\mu)}{\mu + \lambda} = \frac{9\mu B}{3B + \mu} = 2\mu(1+\nu)$

Poisson coefficient: $\nu = \frac{3B - 2\mu}{2(3B + \mu)} = \frac{\lambda}{2(\mu + \lambda)} = \frac{E - 2\mu}{2\mu}$

4. Hooke's Law

Hexagonal elasticity

$$\begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{11} & C_{13} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & C_{44} \end{pmatrix}$$

with $C_{66} = \frac{1}{2}(C_{11} - C_{12})$

$$B = \frac{2C_{11} + C_{33} + 2C_{12} + 4C_{13}}{9}$$

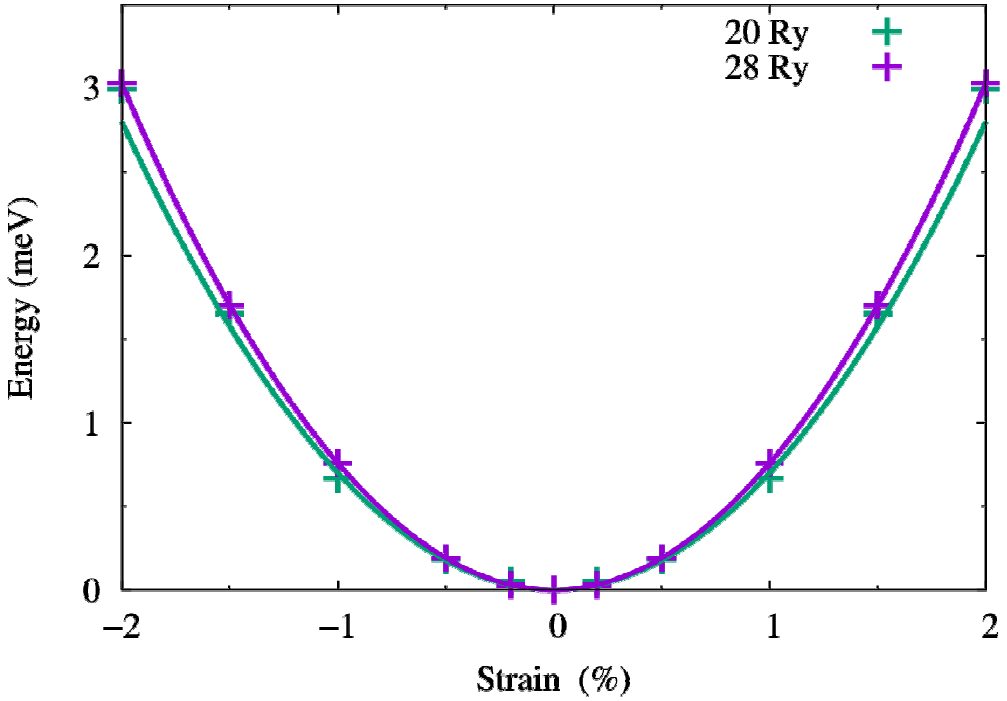
Example: ab initio calculations in Zr

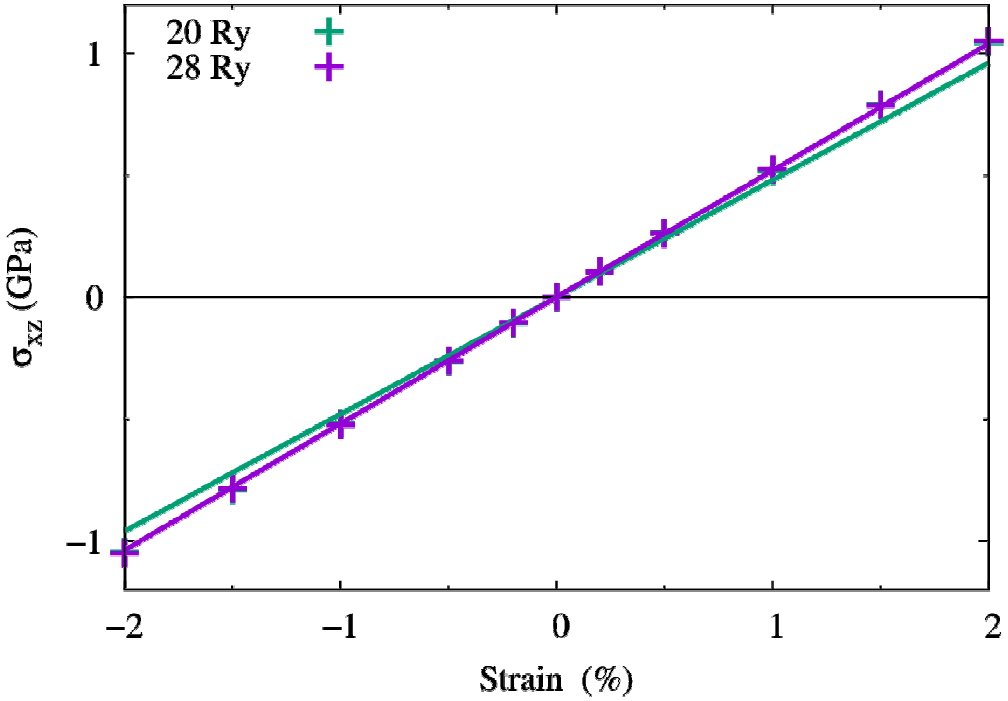
Pwscf:

- DFT GGA
- Ultrasoft pseudopotential ($5s^2\ 4d^2 + 4s^2\ 4p^6$)
- Valence electrons described by plane waves (20 / 28 Ry)
- HCP unit cell (2 atoms)

C_{44} in hcp Zr

$$\boldsymbol{\varepsilon} = \varepsilon \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad \boldsymbol{\sigma} = 2C_{44}\varepsilon \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad \Delta E(\varepsilon) = 2VC_{44}\varepsilon^2$$



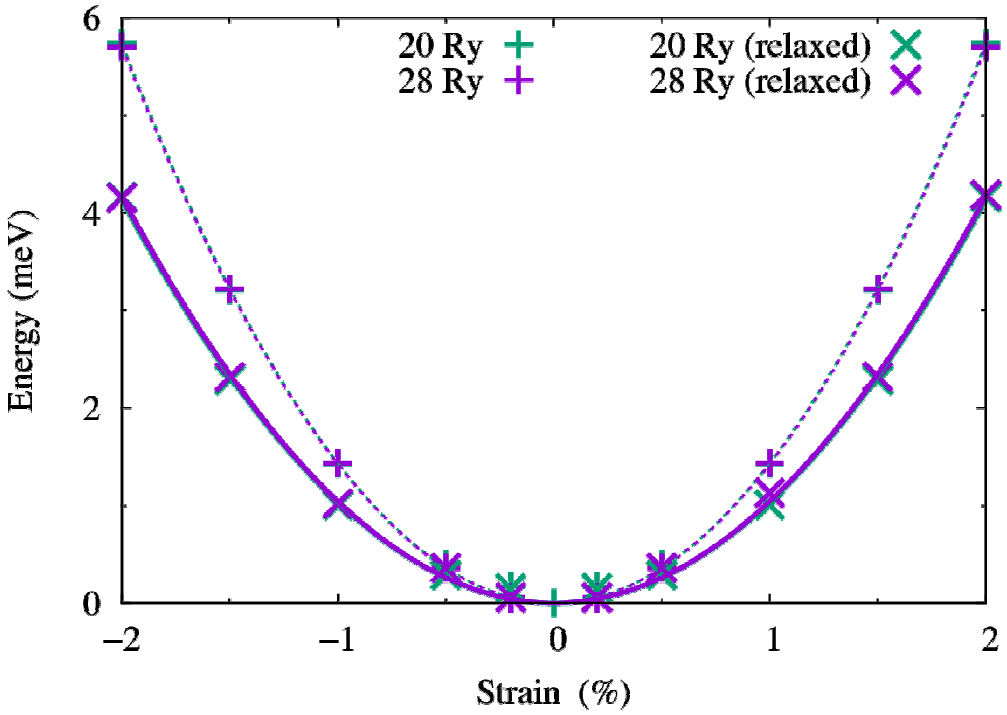


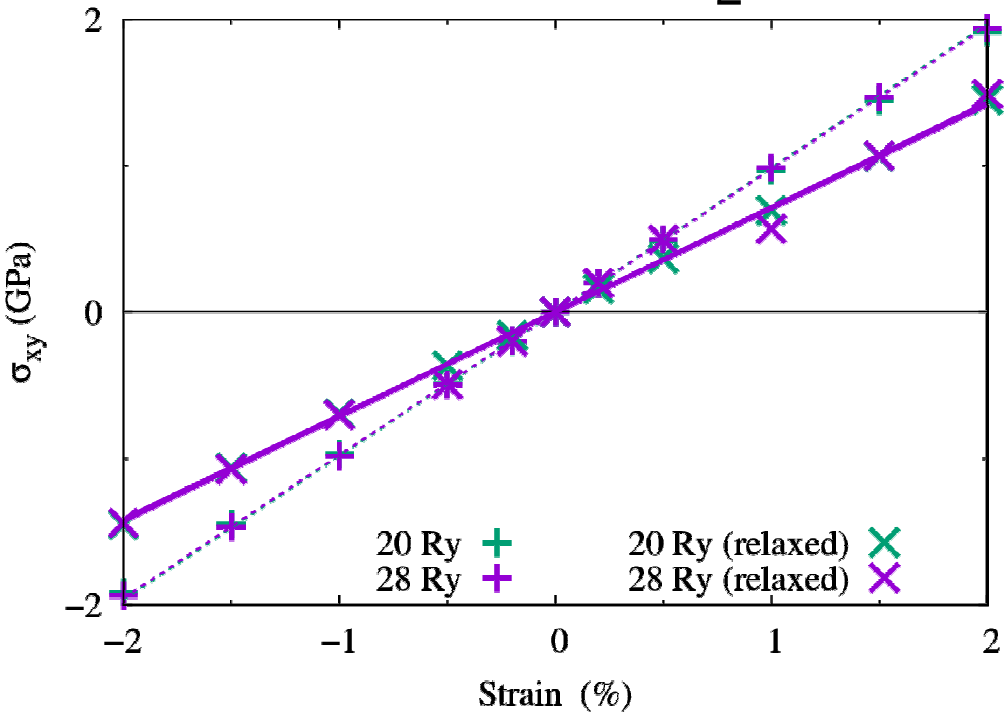
C_{66} in hcp Zr

$$\boldsymbol{\varepsilon} = \varepsilon \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \boldsymbol{\sigma} = 2C_{66}\varepsilon \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\Delta E(\varepsilon) = 2VC_{66}\varepsilon^2$$

with $C_{66} = \frac{1}{2}(C_{11} - C_{12})$

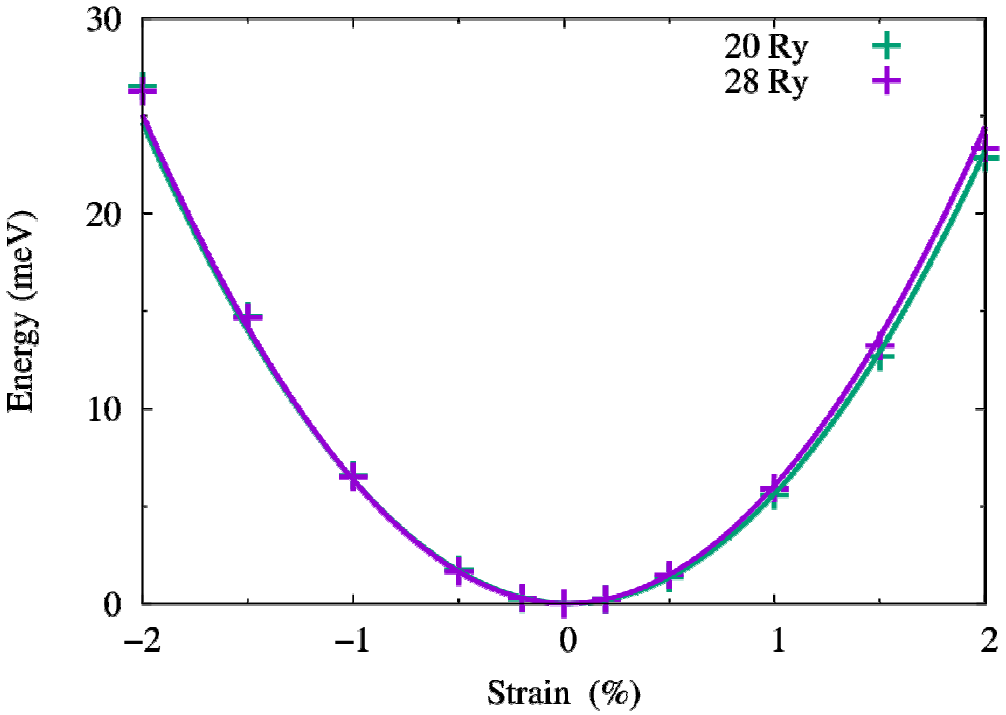


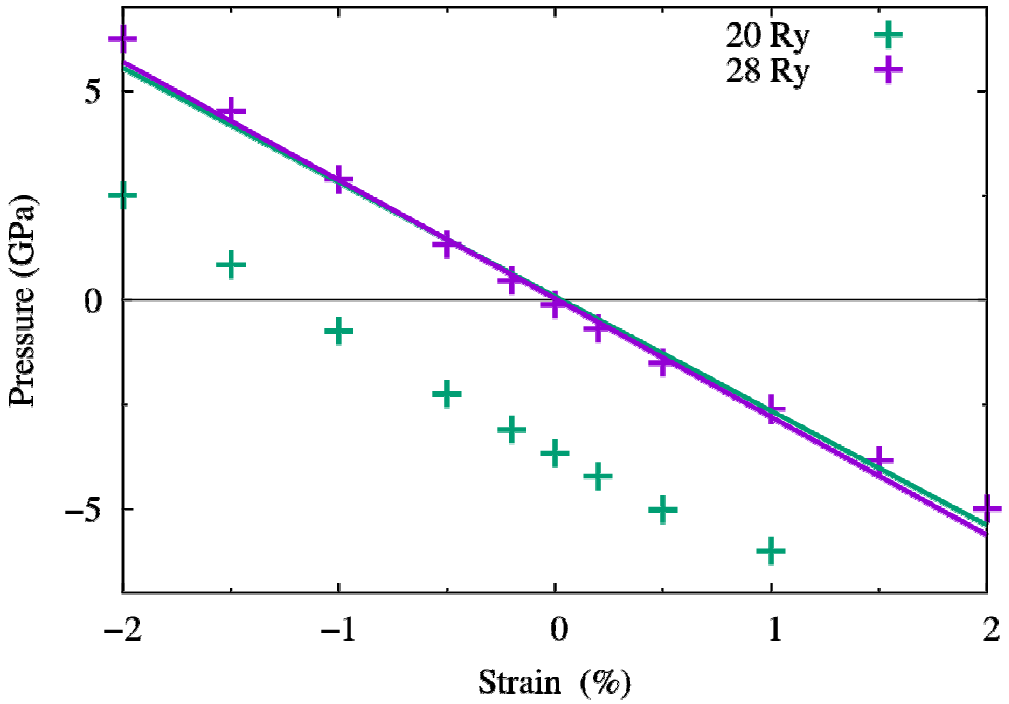


➔ atomic **relaxations** when the crystal symmetry is broken by the strain

B in hcp Zr

$$\boldsymbol{\varepsilon} = \varepsilon \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad P = -\frac{1}{3}\mathrm{Tr}(\boldsymbol{\sigma}) = -3B\varepsilon \qquad \Delta E(\varepsilon) = -\frac{9}{2}VB\varepsilon^2$$





➔ slower convergence of the stress (work with stress differences)

4. Hooke's Law

Hexagonal elasticity $\begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{11} & C_{13} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & C_{44} \end{pmatrix}$ with $C_{66} = \frac{1}{2}(C_{11} - C_{12})$

Example: ab initio calculations in Zr

	Expt.	EAM	SIESTA	PWSCF
a (Å)	3.232 (Ref. 32)	3.234	3.237	3.230
c/a	1.603 (Ref. 32)	1.598	1.613	1.601
C_{11} (GPa)	155.4[a]	142.0	140.0	140.0
C_{33} (GPa)	172.5[a]	168.0	168.0	168.0
C_{12} (GPa)	67.2[a]	75.0	86.0	70.0
C_{13} (GPa)	64.6[a]	76.0	68.0	65.0
C_{44} (GPa)	36.3[a]	44.0	24.0	26.0
C_{66} (GPa)	44.1[a]	33.5	27.0	35.0

5. Equilibrium Equation in Homogeneous Elasticity

$$\frac{\partial \sigma_{ij}}{\partial x_j} + f_i = 0 \qquad \text{with} \quad \sigma_{ij} = C_{ijkl}\varepsilon_{kl} \quad \text{and} \quad \varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

➔ $$\boxed{C_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l} + f_i = 0}$$

\+ $\sigma_{ij} n_j = T_j^a$ and / or $u_i = u_i^a$ at the boundary

Isotropic elasticity

$$(\lambda + \mu)\frac{\partial^2 u_j}{\partial x_i \partial x_j} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + f_i = 0$$

$$(\lambda + \mu)\vec{\nabla}(\vec{\nabla}\cdot\vec{u}) + \mu\,\Delta\vec{u} + \vec{f} = \vec{0}$$

5. Equilibrium Equation in Homogeneous Elasticity

$$C_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l} + f_i = 0 \quad + \quad \sigma_{ij} n_j = T_j^a \quad \text{and / or} \quad u_i = u_i^a \quad \text{at the boundary}$$

Superpostion principle

linear equation (linear elasticity) ➔ solutions can be added
if $\vec{u}^1$ and $\vec{u}^2$ are solutions corresponding to forces $\vec{f}^1$ and $\vec{f}^2$

$$\rightarrow \quad C_{ijkl}\frac{\partial^2 (u_k^{\,1} + u_k^{\,2})}{\partial x_j \partial x_l} + f_i^{\,1} + f_i^{\,2} = 0$$

$$\sigma_{ij} = \sigma_{ij}^{\,1} + \sigma_{ij}^{\,2} = C_{ijkl}\left(\varepsilon_{ij}^{\,1} + \varepsilon_{ij}^{\,2}\right)$$

$$\Delta F = \frac{1}{2} V \left(\sigma_{ij}^{\,1} + \sigma_{ij}^{\,2}\right)\left(\varepsilon_{ij}^{\,1} + \varepsilon_{ij}^{\,2}\right)$$

$$= \frac{1}{2} V \sigma_{ij}^{\,1} \varepsilon_{ij}^{\,1} + \frac{1}{2} V \sigma_{ij}^{\,2} \varepsilon_{ij}^{\,2} + \frac{1}{2} V \left(\sigma_{ij}^{\,1} \varepsilon_{ij}^{\,2} + \sigma_{ij}^{\,2} \varepsilon_{ij}^{\,1}\right)$$

$$= \Delta F^1 + \Delta F^2 + \Delta F^{\text{inter}}$$

Elastic interaction energy
(between defects, …)

$$\Delta F^{\text{inter}} = V \sigma_{ij}^{\,1} \varepsilon_{ij}^{\,2} = V \sigma_{ij}^{\,2} \varepsilon_{ij}^{\,1}$$

5. Equilibrium Equation in Homogeneous Elasticity

$$C_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l} + f_i = 0 \quad + \quad \sigma_{ij} n_j = T_j^{\mathrm{a}} \quad \text{and / or} \quad u_i = u_i^{\mathrm{a}} \quad \text{at the boundary}$$

Superpostion principle:

➔ **Green's function**: solution to a unit point force (Dirac delta function)

$$C_{ijkl}\frac{\partial^2 G_{kn}}{\partial x_j \partial x_l} + \delta_{in}\delta(\vec{x}) = 0 \quad \text{with} \quad \delta(\vec{x}) = \begin{cases} 0 \text{ if } \vec{x} \neq \vec{0} \\ \infty \text{ if } \vec{x} = \vec{0} \end{cases}$$

$G_{kn}(\vec{r})$: tensor field giving the displacement along the x_k axis of a unit point force applied along the x_n at the origin

Solution to the force distribution $\int \vec{f}(\vec{x}')\mathrm{d}\vec{x}'$

$$u_k(\vec{x}) = \int G_{kn}(\vec{x} - \vec{x}')\, f_n(\vec{x}')\mathrm{d}\vec{x}'$$

$$\sigma_{ij}(\vec{x}) = C_{ijkl}\int G_{kn,l}(\vec{x} - \vec{x}')\, f_n(\vec{x}')\mathrm{d}\vec{x}'$$

with $G_{kn,l} = \dfrac{\partial G_{kn}}{\partial x_l}$

5. Equilibrium Equation in Homogeneous Elasticity

Green's function

- isotropic elasticity: $$G_{kn}(\vec{x}) = \frac{1}{16\pi\mu(1-\nu)|\vec{x}|}\left[(3-4\nu)\delta_{ij} + \frac{x_k x_n}{|\vec{x}|^2}\right]$$

- anisotropic elasticity:

  analytical expression only for transverse isotropy (hexagonal)
  ➔ numerical evaluation needed

  D. M. Barnett, Phys. Status Solidi B **49**, 741 (1972).

  but the radial dependence does not vary

$$G_{kn}(\vec{r}) = \frac{1}{r} g(\theta,\phi)$$

$$G_{kn,i}(\vec{r}) = \frac{1}{r^2} h(\theta,\phi)$$

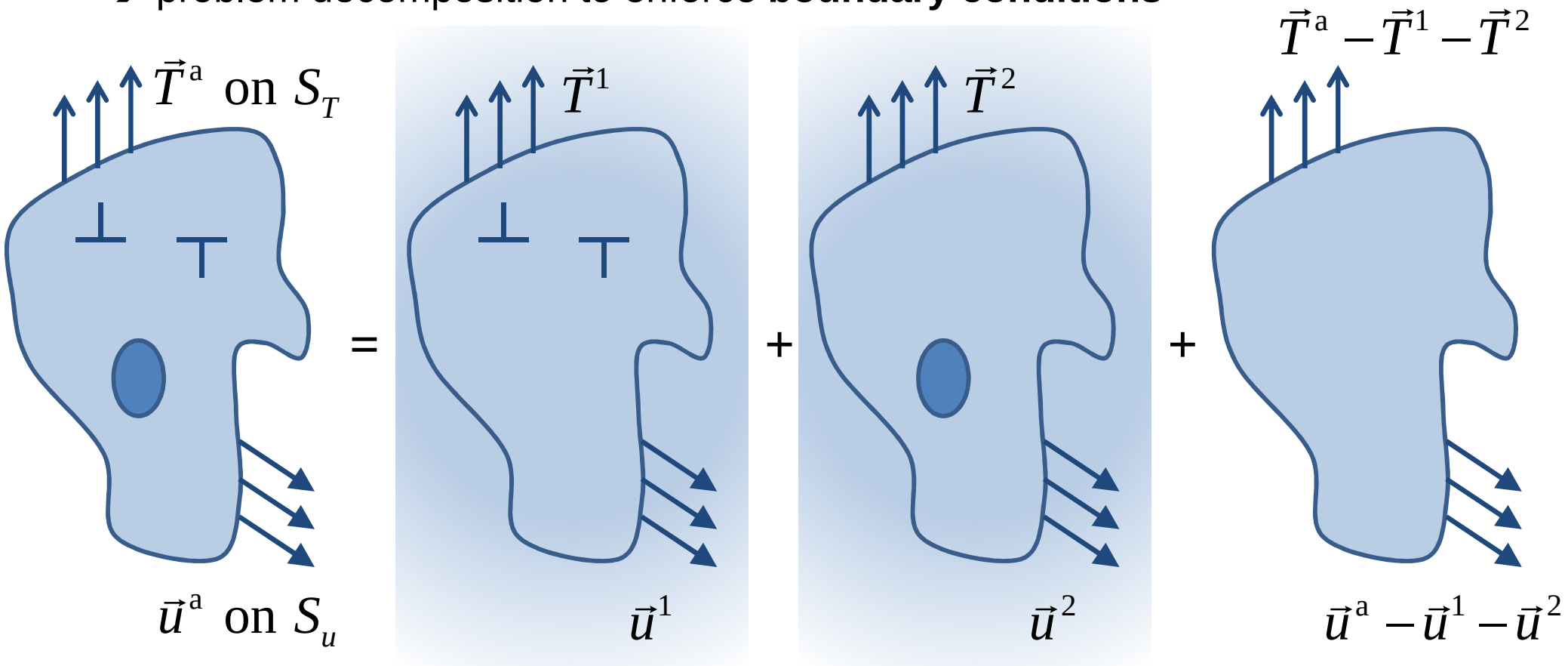
$$G_{kn,ij}(\vec{r}) = \frac{1}{r^3} f(\theta,\phi)$$

5. Equilibrium Equation in Homogeneous Elasticity

$$C_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l} + f_i = 0 \quad + \quad \sigma_{ij} n_j = T_j^{\mathrm{a}} \quad \text{and / or} \quad u_i = u_i^{\mathrm{a}} \quad \text{at the boundary}$$

Superpostion principle:

➔ problem decomposition to enforce **boundary conditions**



E. van der Giessen and A. Needleman, Modelling Simul. Mater. Sci. Eng. **3**, 689 (1995).

5. Equilibrium Equation in Homogeneous Elasticity

$$C_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l} + f_i = 0 \quad + \quad \sigma_{ij} n_j = T_j^{\mathrm{a}} \quad \text{and / or} \quad u_i = u_i^{\mathrm{a}} \quad \text{at the boundary}$$

Fourier transform method

linear partial differential equation ➔ solutions in reciprocal space

$$\vec{u}(\vec{r}) = \int \vec{U}(\vec{q})\, \mathrm{e}^{-\mathrm{i}\,\vec{q}\cdot\vec{r}}\, \mathrm{d}\vec{q} \quad \text{and} \quad \vec{f}(\vec{r}) = \int \vec{F}(\vec{q})\, \mathrm{e}^{-\mathrm{i}\,\vec{q}\cdot\vec{r}}\, \mathrm{d}\vec{q}$$

➔ $-C_{ijkl} q_j q_l U_k + F_i = 0$

$$U_k = (qq)^{-1}_{ki} F_i \quad \text{with} \quad (qq)_{ik} = C_{ijkl} q_j q_l$$

Fourier transform of Green's function: $(qq)^{-1}_{ki}$

$$\boldsymbol{\sigma}(\vec{r}) = \int \boldsymbol{\Sigma}(\vec{q})\, \mathrm{e}^{-\mathrm{i}\,\vec{q}\cdot\vec{r}}\, \mathrm{d}\vec{q} \quad \text{where} \quad \Sigma_{ij} = -\mathrm{i} C_{ijkl} q_l (qq)^{-1}_{kn} F_n$$

complex microstructure (phase field, polycrystal homogenization), but

- **periodic** boundary conditions
- spatial **resolution** d in a box of dimension L limited by the number N of nodes of the FFT grid: $N = L/d$

T. Mura, Micromechanics of Defects in Solids (1987).

II. Inclusions, Inhomogeneities and Point Defects

1. Spherical inclusion
2. Eshelby's inclusion
3. Inclusion and applied stress
4. Point defect
5. Carbon - dislocation interaction in iron
6. Isolated point-defect in ab initio calculations
7. Inhomogeneity and polarizability

References:

- J. D. Eshelby, Proc. Roy. Soc. Lond. A **241**, 376 (1957); *ibid* **252**, 561 (1959).
- G. Leibfried and N. Breuer, Point Defects in Metals I 81 (1978).
- D. J. Bacon, D. M. Barnett and R. O. Scattergood, Prog. Mater. Sci. **23**, 51 (1980).
- R. W. Balluffi, Introduction to Elasticity Theory for Crystal Defects (2012).
- C. Weinberger, W. Cai and D. Barnett, *Elasticity of Microscopic Structures*, Standford Univ. lecture notes (2005).

Isotropic elasticity in spherical symmetry

spherical symmetry $\vec{u}(\vec{r}) = u(r)\vec{e}_r$

isotropic elasticity $(\lambda+\mu)\vec{\nabla}(\vec{\nabla}\cdot\vec{u})+\mu\,\Delta\vec{u}+\vec{f}=\vec{0}$

no body force

$$\frac{\partial}{\partial r}\left(\frac{\partial u}{\partial r}+\frac{2u}{r}\right)=0 \quad \rightarrow \quad \boxed{u(r)=A\,r+\frac{B}{r^2}}$$

$$\boldsymbol{\varepsilon}=\vec{\nabla}\otimes\vec{u}$$

$$\varepsilon_{rr}=\frac{\partial u}{\partial r}=A-2\frac{B}{r^3} \qquad \varepsilon_{\theta\theta}=\varepsilon_{\phi\phi}=\frac{u}{r}=A+\frac{B}{r^3} \qquad \frac{\Delta V}{V}=3A$$

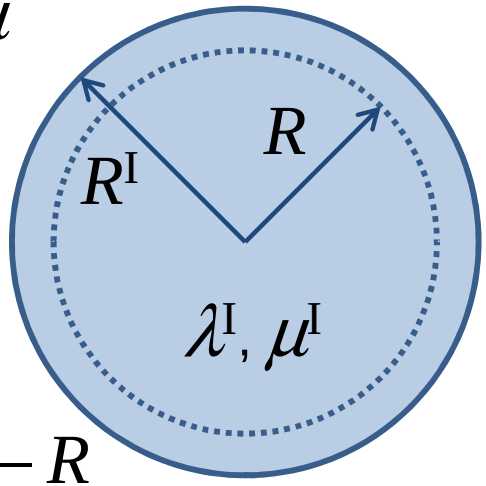
$$\sigma_{ij}=\left[\lambda\delta_{ij}\delta_{kl}+\mu(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\right]\varepsilon_{kl}$$

$$\sigma_{rr}=(3\lambda+2\mu)A-4\mu\frac{B}{r^3} \qquad \sigma_{\theta\theta}=\sigma_{\phi\phi}=(3\lambda+2\mu)A+2\mu\frac{B}{r^3}$$

$$P=-3(\lambda+2\mu)A$$

Density of elastic energy: $f=\frac{3}{2}(3\lambda+2\mu)A^2+6\mu\frac{B^2}{r^6}$

Spherical inclusion: infinite system



$$\delta R = R^{\mathrm{I}} - R$$

Inside the inclusion

$$u_{\mathrm{I}}(r) = A^{\mathrm{I}} r$$

$$\varepsilon^{\mathrm{I}} = A^{\mathrm{I}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

homogeneous compression

Outside the inclusion

$$u(r) = \frac{B}{r^2}$$

$$\varepsilon = \frac{B}{r^3} \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

pure shear

Continuity at the interface

$$\begin{cases} R^{\mathrm{I}} + u^{\mathrm{I}}(R^{\mathrm{I}}) = R + u(R) \\ \sigma^{\mathrm{I}}(R^{\mathrm{I}}) = \sigma(R) \end{cases}$$

$$\begin{cases} R^{\mathrm{I}} + A^{\mathrm{I}} R^{\mathrm{I}} = R + \dfrac{B}{R^2} \\ \left(3\lambda^{\mathrm{I}} + 2\mu^{\mathrm{I}}\right) A^{\mathrm{I}} = -4\mu \dfrac{B}{R^3} \end{cases}$$

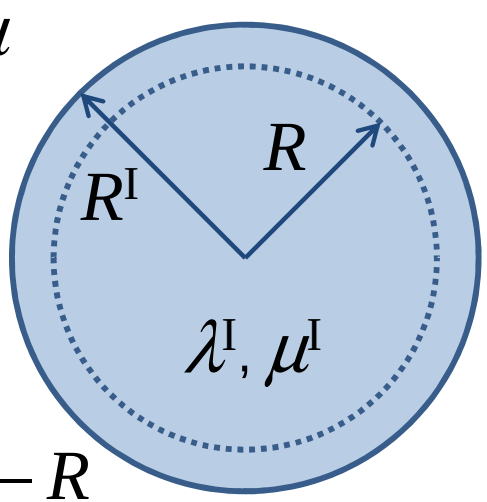
$$A^{\mathrm{I}} = -\frac{4\mu}{3\lambda^{\mathrm{I}} + 2\mu^{\mathrm{I}} + 4\mu} \frac{\delta R}{R}$$

$$B = \frac{3\lambda^{\mathrm{I}} + 2\mu^{\mathrm{I}}}{3\lambda^{\mathrm{I}} + 2\mu^{\mathrm{I}} + 4\mu} R^3 \frac{\delta R}{R}$$

1. Spherical Inclusion

Spherical inclusion: infinite system

$$u(r) = A\,r + \frac{B}{r^2}$$



$$\delta R = R^{\mathrm{I}} - R$$

Inside the inclusion

$$u_{\mathrm{I}}(r) = A^{\mathrm{I}} r$$

$$\varepsilon^{\mathrm{I}} = A^{\mathrm{I}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

homogeneous compression

Outside the inclusion

$$u(r) = \frac{B}{r^2}$$

$$\varepsilon = \frac{B}{r^3} \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

pure shear

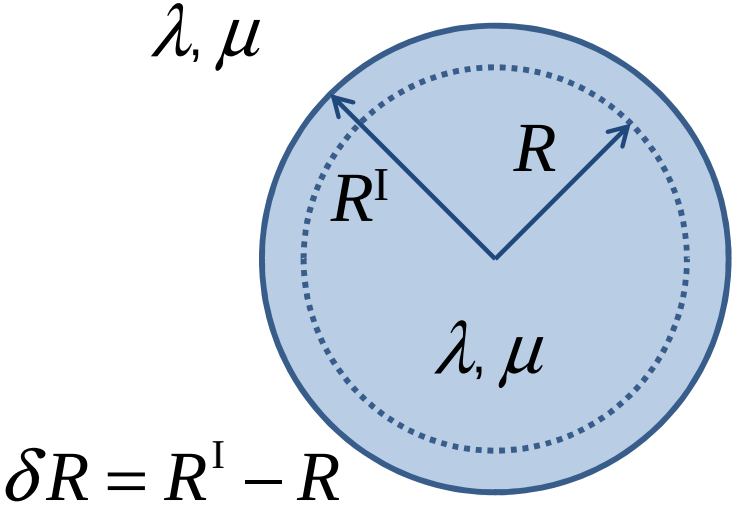
Elastic energy:

$$F = \frac{3}{2}(3\lambda^{\mathrm{I}} + 2\mu^{\mathrm{I}})A^{\mathrm{I}2}\frac{4}{3}\pi R^3 + \int_R^{\infty} 6\mu \frac{B^2}{r^6} 4\pi r^2 \mathrm{d}r$$

$$F = \frac{6\mu(3\lambda^{\mathrm{I}} + 2\mu^{\mathrm{I}})}{(3\lambda^{\mathrm{I}} + 2\mu^{\mathrm{I}} + 4\mu)} \Omega^{\mathrm{I}} \left(\frac{\delta R}{R}\right)^2$$

with $\Omega^{\mathrm{I}} = \frac{4}{3}\pi R^3$

Homogeneous spherical inclusion : infinite system



$$\delta R = R^{\mathrm{I}} - R$$

Inside the inclusion

$$u_{\mathrm{I}}(r) = A^{\mathrm{I}} r$$

$$\varepsilon^{\mathrm{I}} = A^{\mathrm{I}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$A^{\mathrm{I}} = -\frac{4\mu}{3(\lambda+2\mu)} \frac{\delta R}{R}$$

Outside the inclusion

$$u(r) = \frac{B}{r^2}$$

$$\varepsilon = \frac{B}{r^3} \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$B = \frac{3\lambda+2\mu}{3(\lambda+2\mu)} R^3 \frac{\delta R}{R}$$

Eigenstrain: inclusion strain before matrix relaxation

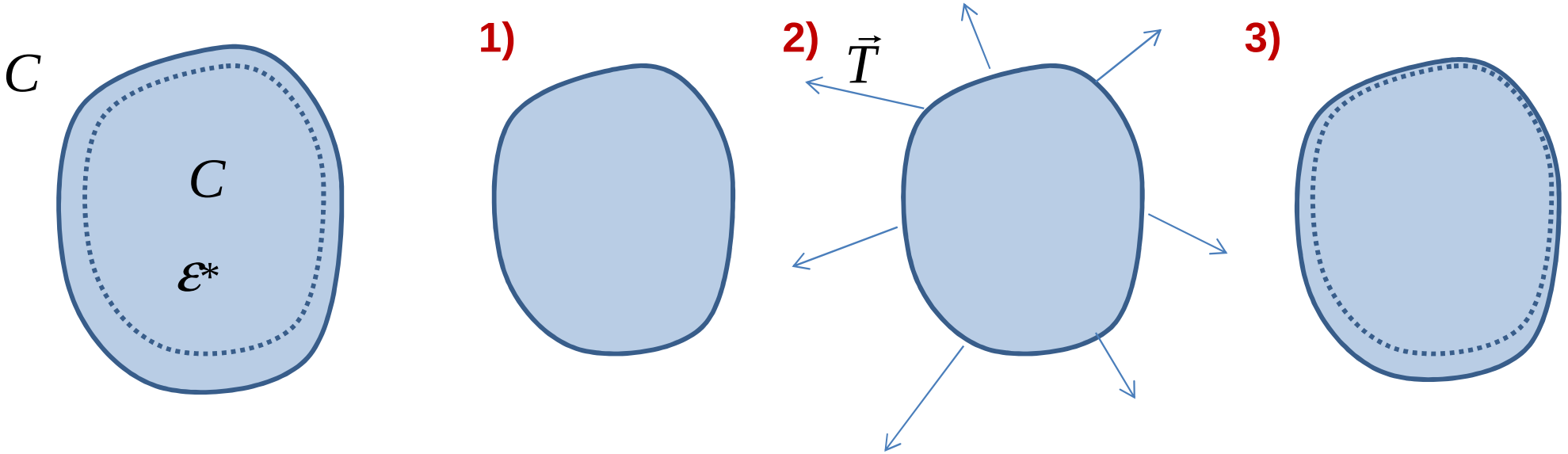
$$\varepsilon^* = -\frac{\delta R}{R} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \rightarrow \quad \boldsymbol{\varepsilon}^{\mathrm{I}} = \frac{4\mu}{3(\lambda+2\mu)} \boldsymbol{\varepsilon}^*$$

Elastic energy:

$$F = \frac{2\mu(3\lambda+2\mu)}{(\lambda+2\mu)} \Omega^{\mathrm{I}} \left(\frac{\delta R}{R}\right)^2 = \frac{3}{2}(3\lambda+2\mu)\Omega^{\mathrm{I}} \left(\varepsilon^*\right)^2 \left[1 - \frac{3\lambda+2\mu}{3(\lambda+2\mu)}\right]$$

$$F = \frac{1}{2} B \frac{\left(\delta\Omega^{\mathrm{I}}\right)^2}{\Omega^{\mathrm{I}}} \left[1 - \frac{3\lambda+2\mu}{3(\lambda+2\mu)}\right]$$

2. Eshelby's Inclusion



1) Strain the inclusion to fit the hole

elastic field in the inclusion $\boldsymbol{\varepsilon}^{\mathrm{I}} = \boldsymbol{\varepsilon}^{*}$ $\boldsymbol{\sigma}^{\mathrm{I}} = \mathbf{C} : \boldsymbol{\varepsilon}^{*}$

elastic field outside $\boldsymbol{\varepsilon} = \mathbf{0}$ $\boldsymbol{\sigma} = \mathbf{0}$

2) Weld the inclusion in the hole

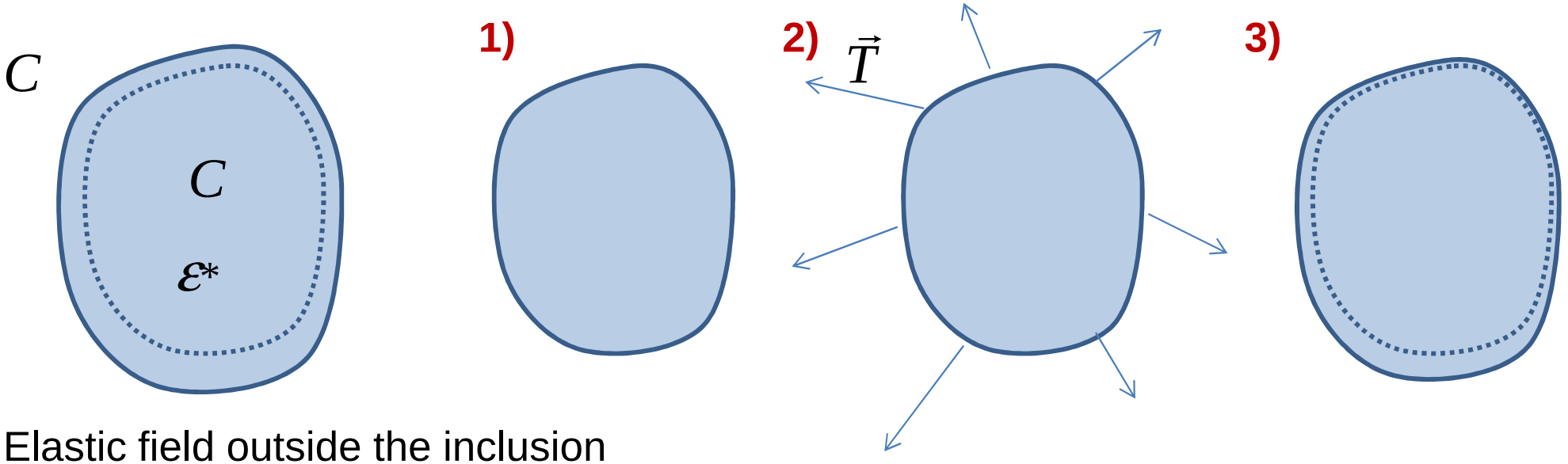
➔ need to apply body force along the surface to compensate tractions caused by inclusion stress

$$\vec{T} = -\int \mathbf{C} : \boldsymbol{\varepsilon}^{*} \, \mathrm{d}\vec{S}$$

3) Relax surface traction

J. D. Eshelby, Proc. Roy. Soc. Lond. A **241**, 376 (1957); **252**, 561 (1959).

2. Eshelby's Inclusion



Elastic field outside the inclusion

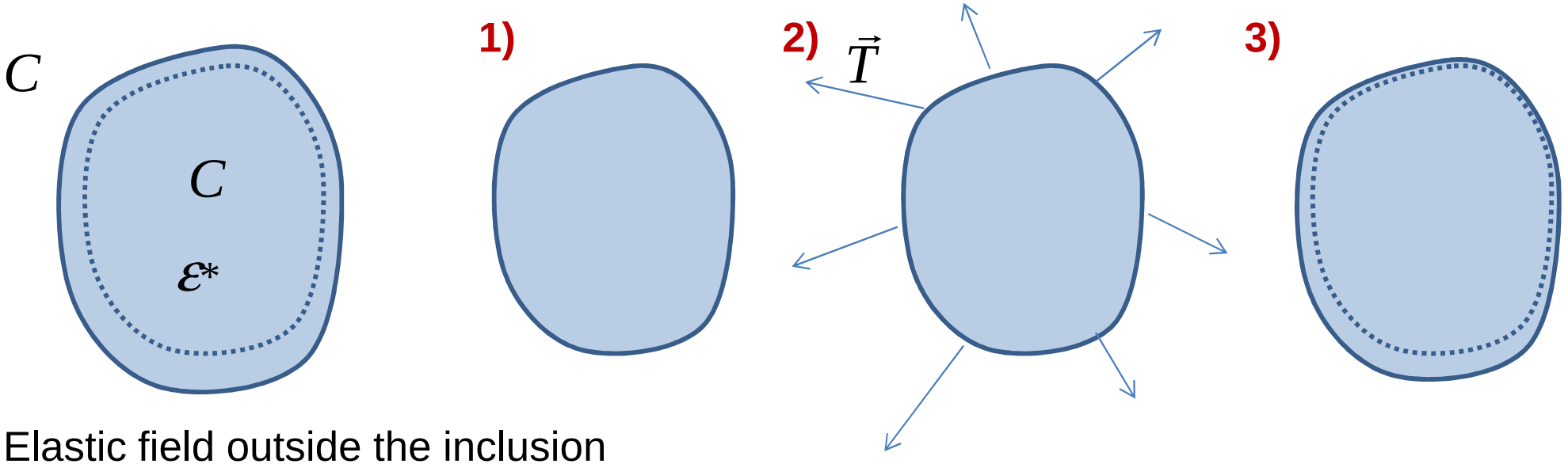
$$u_i(\vec{x}) = \oint_S G_{ij}(\vec{x}-\vec{x}')T_j(\vec{x}')\mathrm{d}S'$$

$$= -\oint_S G_{ij}(\vec{x}-\vec{x}')\sigma^*_{jk}(\vec{x}')n_k(\vec{x}')\mathrm{d}S' \qquad \text{with} \qquad \sigma^*_{jk} = C_{jkmn}\varepsilon^*_{mn}$$

$$= -\int_{\Omega^I} \frac{\partial}{\partial x_k}\left[G_{ij}(\vec{x}-\vec{x}')\sigma^*_{jk}(\vec{x}')\right]\mathrm{d}V'$$

$$= -\int_{\Omega^I} G_{ij,k}(\vec{x}-\vec{x}')\sigma^*_{jk}(\vec{x}')\mathrm{d}V' \qquad \text{because} \qquad \frac{\partial \sigma^*_{jk}}{\partial x_k} = 0$$

2. Eshelby's Inclusion



Elastic field outside the inclusion

$$u_i(\vec{x}) = -\int_{\Omega^I} G_{ij,k}(\vec{x}-\vec{x}')\sigma^*_{jk}(\vec{x}')\mathrm{d}V' \qquad \text{with} \qquad \sigma^*_{jk} = C_{jkmn}\varepsilon^*_{mn}$$

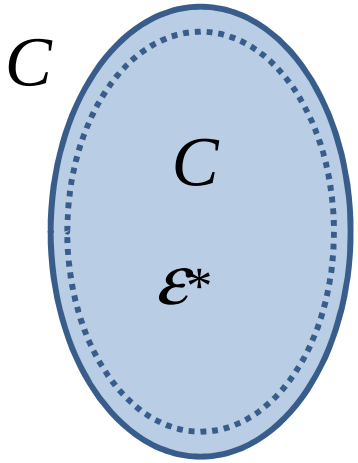
$$\varepsilon_{mn}(\vec{x}) = -\int_{\Omega^I} G_{mj,nk}(\vec{x}-\vec{x}')\sigma^*_{jk}(\vec{x}')\mathrm{d}V'$$

$$\sigma_{pq}(\vec{x}) = -C_{pqmn}\int_{\Omega^I} G_{mj,nk}(\vec{x}-\vec{x}')\sigma^*_{jk}(\vec{x}')\mathrm{d}V'$$

Elastic field inside the inclusion: add the eigenstrain

2. Eshelby's Inclusion

Ellipsoidal inclusion



If the eigenstrain is homogeneous, then the strain inside the inclusion is also homogeneous

$$\varepsilon_{ij}^{\mathrm{I}} = S_{ijkl}^{\mathrm{E}} \varepsilon_{kl}^{*}$$

Eshelby tensor:

$$S_{ijmn}^{\mathrm{E}} = \frac{1}{2} C_{klmn} \int_{\Omega^{\mathrm{I}}} \left[G_{ik,jl}(\vec{x}) + G_{jk,il}(\vec{x}) \right] \mathrm{d}V$$

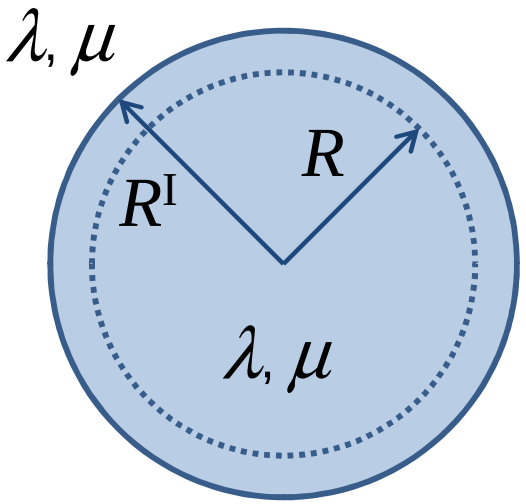
(minor symmetries but no major symmetry)

Elastic energy:

$$F = \frac{1}{2} \Omega^{\mathrm{I}} C_{ijkl} \varepsilon_{ij}^{*} \varepsilon_{ij}^{*} - \frac{1}{2} \Omega^{\mathrm{I}} C_{ijkl} S_{klmn}^{\mathrm{E}} \varepsilon_{ij}^{*} \varepsilon_{mn}^{*}$$

$$= \frac{1}{2} \Omega^{\mathrm{I}} C_{ijkl} \left(\delta_{km} \delta_{ln} - S_{klmn}^{\mathrm{E}} \right) \varepsilon_{ij}^{*} \varepsilon_{mn}^{*}$$

Homogeneous spherical inclusion : **infinite** system



Inside the inclusion

$$u_{\mathrm{I}}(r) = A^{\mathrm{I}} r$$

$$\varepsilon^{\mathrm{I}} = A^{\mathrm{I}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$A^{\mathrm{I}} = -\frac{4\mu}{3(\lambda+2\mu)} \frac{\delta R}{R}$$

Outside the inclusion

$$u(r) = \frac{B}{r^2}$$

$$\varepsilon = \frac{B}{r^3} \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$B = \frac{3\lambda+2\mu}{3(\lambda+2\mu)} R^3 \frac{\delta R}{R}$$

Homogeneous spherical inclusion : **finite** system

the displacement cancel in R_{e} (no external strain)

➔ superposition of a homogeneous strain ε_0

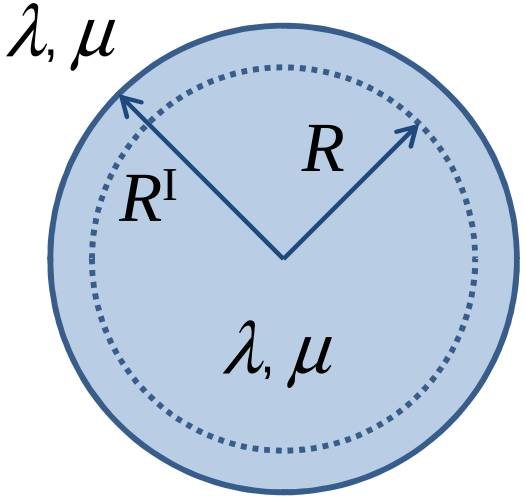
$$u(R^{\mathrm{E}}) = \frac{B}{R^{\mathrm{E}2}} + \varepsilon_0 R^{\mathrm{E}} = 0$$

$$\varepsilon^{\mathrm{I}} = \left(A^{\mathrm{I}} - \frac{B}{R^{\mathrm{E}3}} \right) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\varepsilon = \frac{B}{r^3} \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{B}{R^{\mathrm{E}3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

➔ variation of the elastic energy (image forces)

Homogeneous spherical inclusion : **finite** system



Inside the inclusion

$$u_{\mathrm{I}}(r) = \left(A^{\mathrm{I}} - \frac{B}{R^{\mathrm{E}3}} \right) r$$

$$\boldsymbol{\varepsilon}^{\mathrm{I}} = \left(A^{\mathrm{I}} - \frac{B}{R^{\mathrm{E}3}} \right) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Outside the inclusion

$$u(r) = B \left(\frac{1}{r^2} - \frac{r}{R^{\mathrm{E}3}} \right)$$

$$\boldsymbol{\varepsilon} = \frac{B}{r^3} \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{B}{R^{\mathrm{E}3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Interaction with an applied strain : $\varepsilon^{\mathrm{A}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ $A^{\mathrm{I}} = -\frac{4\mu}{3(\lambda+2\mu)} \frac{\delta R}{R}$ $B = \frac{3\lambda+2\mu}{3(\lambda+2\mu)} R^3 \frac{\delta R}{R}$

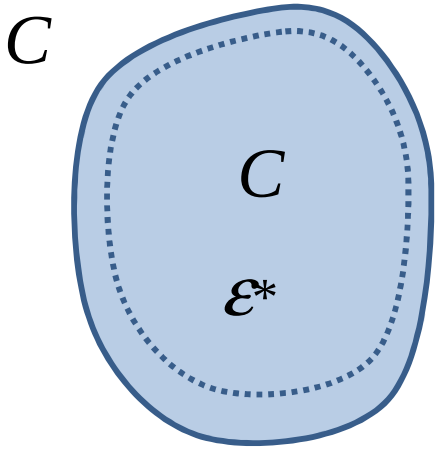
Interaction between 2 elastic fields (superposition) $F^{\mathrm{inter}} = V \sigma_{ij}^{\ 1} \varepsilon_{ij}^{\ 2} = V \sigma_{ij}^{\ 2} \varepsilon_{ij}^{\ 1}$

$$F^{\mathrm{inter}} = \frac{4}{3} \pi R^3 3(3\lambda+2\mu) A^{\mathrm{I}} \varepsilon^{\mathrm{A}} - \frac{4}{3} \pi R^{\mathrm{E}3} 3(3\lambda+2\mu) \frac{B}{R^{\mathrm{E}3}} \varepsilon^{\mathrm{A}}$$

$$F^{\mathrm{inter}} = -\Omega^{\mathrm{I}} 3(3\lambda+2\mu) \frac{\delta R}{R} \varepsilon^{\mathrm{A}}$$

$$F^{\mathrm{inter}} = -3\Omega^{\mathrm{I}} \varepsilon^{*} P^{\mathrm{A}} \quad \text{with} \quad P^{\mathrm{A}} = -(3\lambda+2\mu)\varepsilon^{\mathrm{A}}$$

Eshelby inclusion



Interaction with an applied strain

$$F^{\text{inter}} = -\int_{\Omega^{\text{I}}} C_{ijkl}\varepsilon^{*}_{ij}(\vec{x})\varepsilon^{\text{A}}_{kl}(\vec{x})\text{d}V$$

for an homogeneous eigenstrain

$$F^{\text{inter}} = -C_{ijkl}\varepsilon^{*}_{ij}\int_{\Omega^{\text{I}}} \varepsilon^{\text{A}}_{kl}(\vec{x})\text{d}V$$

Infinitesimal Inclusion :

interest only in the far-field elastic range

➔ limit of small inclusion volume $\Omega_{\mathrm{I}} \to 0$

assumption: homogeneous inclusion (not necessary because average eigenstrain)

$$\sigma^*_{jk} = C_{jkmn}\varepsilon^*_{mn}$$

Elastic field outside the inclusion

$$u_i(\vec{x}) = -\int_{\Omega^{\mathrm{I}}} G_{ij,k}(\vec{x}-\vec{x}')\sigma^*_{jk}(\vec{x}')\mathrm{d}V'$$

➔ $$u_i(\vec{x}) = -G_{ij,k}(\vec{x})\Omega^{\mathrm{I}}\sigma^*_{jk} \qquad \propto \frac{1}{r^2}$$

$$\sigma_{pq}(\vec{x}) = -C_{pqmn}\int_{\Omega^{\mathrm{I}}} G_{mj,nk}(\vec{x}-\vec{x}')\sigma^*_{jk}(\vec{x}')\mathrm{d}V'$$

➔ $$\sigma_{pq}(\vec{x}) = -C_{pqmn}G_{mj,nk}(\vec{x})\Omega^{\mathrm{I}}\sigma^*_{jk} \propto \frac{1}{r^3}$$

Interaction with an applied strain

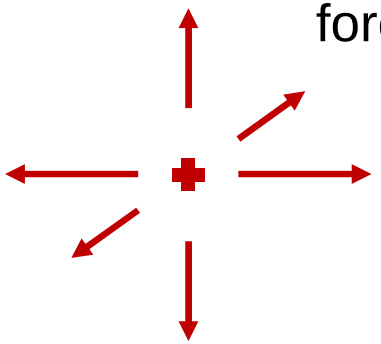
$$F^{\mathrm{inter}} = \int_{\Omega^{\mathrm{I}}} C_{ijkl}\varepsilon^*_{ij}(\vec{x})\varepsilon^{\mathrm{A}}_{kl}(\vec{x})\mathrm{d}V \quad \rightarrow \quad F^{\mathrm{inter}} = \Omega^{\mathrm{I}}\sigma^*_{ij}\varepsilon^{\mathrm{A}}_{ij}(\vec{0})$$

Infinitesimal inclusion fully characterized by $\boxed{\Omega^{\mathrm{I}}\sigma^*_{ij} = \Omega^{\mathrm{I}}C_{ijkl}\varepsilon^*_{kl}}$

(strain source)

Dipole :

Point defect modeled as an equilibrated distribution of point forces:



force $\vec{F}^n$ acting in $\vec{a}^n$

Equilibrium ➔ Resultant : $\sum_n \vec{F}^n = \vec{0}$

➔ Net torque : $\sum_n \vec{F}^n \times \vec{a}^n = \vec{0}$

Displacement created by the point defect: $u_i(\mathbf{r}) = \sum_n G_{ij}(\vec{r} - \vec{a}^n) F_j^n$

Long range displacement: $r \gg \left\| \vec{a}^n \right\|$

$$u_i(\vec{r}) = G_{ij}(\vec{r}) \sum_n F_j^n - \frac{\partial G_{ij}(\vec{r})}{\partial r_k} \sum_n F_j^n a_k^n + \dots$$

$= 0$ (equilibrium: no force resultant)

$P_{jk} = \sum_n F_j^n a_k^n$: elastic dipole modeling the point defect

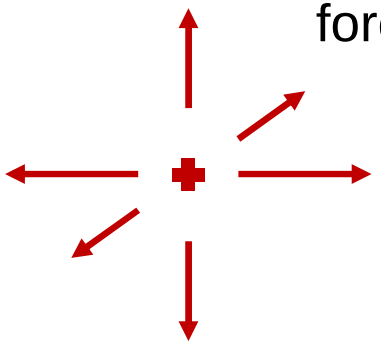
(first moment of the force distribution)

symmetric tensor (equilibrium: no torque)

➔ $u_i(\vec{r}) = -G_{ij,k}(\vec{r}) P_{jk}$ and $\sigma_{ij}(\vec{r}) = -C_{ijkl} G_{km,nl}(\vec{r}) P_{mn}$

Dipole :

Point defect modeled as an equilibrated distribution of point forces:



force $\vec{F}^n$ acting in $\vec{a}^n$

$$P_{jk} = \sum_n F_j^n a_k^n$$

Interaction with an applied elastic field:

$$F^{\text{inter}} = -\sum_n F_k^n \, u_k^{\text{A}}(\vec{a}^n)$$

Limited expansion:

$$F^{\text{inter}} = u_k^{\text{A}}(\vec{0}) \sum_n F_k^n - u_{k,l}^{\text{A}}(\mathbf{0}) \sum_n F_k^n a_l^n + \ldots$$

$$= -\varepsilon_{kl}^{\text{A}}(\vec{0}) P_{kl} + \ldots$$

D. J. Bacon, D. M. Barnett and R. O. Scattergood, Prog. Mater. Sci. **23**, 51 (1980).

Point defects:

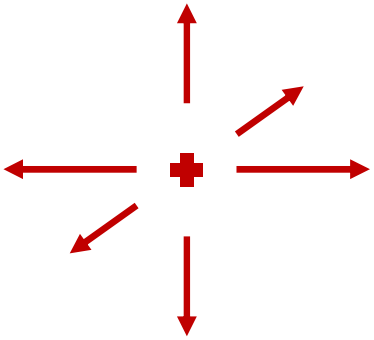
2 equivalent modelds:

- Eshelby infinitesimal inclusion
- elastic dipole

$$\boxed{\Omega^{\text{I}} \varepsilon_{ij}^{*} = C_{ijkl}^{-1} P_{kl}}$$

$$F^{\text{inter}} = -\varepsilon_{kl}^{\text{A}}(\vec{0}) P_{kl} = -\sigma_{kl}^{\text{A}}(\vec{0}) \Omega^{\text{I}} \varepsilon_{kl}^{*}$$

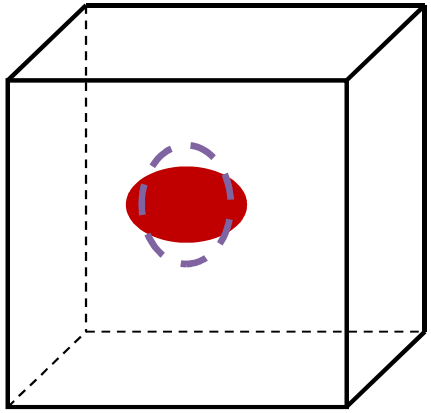
Point defect in an elastic body: 2 equivalent models



- Eshelby infinitesimal inclusion
- elastic dipole

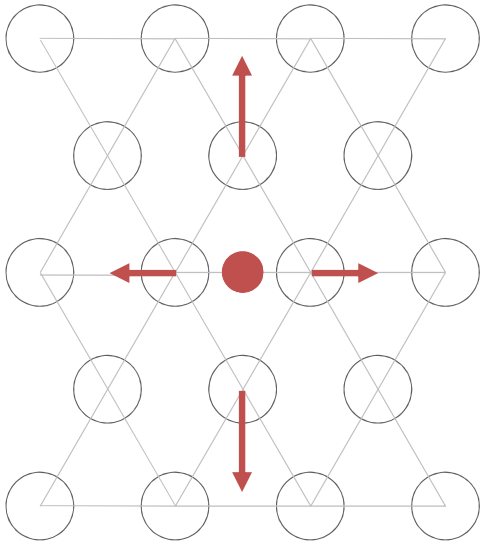
$$\Omega^{\mathrm{I}} \varepsilon_{ij}^{*} = C^{-1}_{ijkl} P_{kl}$$

$$F^{\mathrm{inter}} = -\varepsilon^{\mathrm{A}}_{kl}(\vec{0}) P_{kl} = -\sigma^{\mathrm{A}}_{kl}(\vec{0}) \Omega^{\mathrm{I}} \varepsilon^{*}_{kl}$$



+ infinitesimal dislocation loop

Microscopic elasticity theory (Khachaturyan, Cook, De Fontaine)



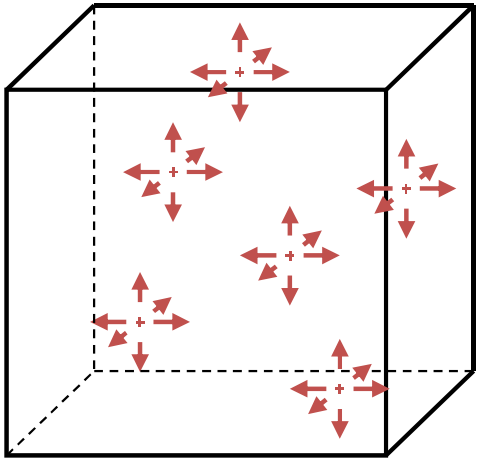
Point defect modeled by Kanzaki forces $\mathbf{F}^{n}$

Only the first moment in dipole approach

Crystal answers through its force-constant matrices corresponding to its whole phonon spectrum

Elastic continuum corresponds to the long wavelength limit (C_{ijkl} ~ slope of the phonon dispersion in Γ)

Determination of the elastic dipole from atomistic simulations



Volume V

- containing n^{PD} point defects P_{ij}
- submitted to a homogeneous strain ε_{ij}

Elastic energy:

$$E = n^{PD}E^{PD} + E^{PD}_{inter} + \frac{1}{2}VC_{ijkl}\varepsilon_{ij}\varepsilon_{kl} - n^{PD}P_{ij}\varepsilon_{ij}$$

E^{PD} : point defect self energy

E^{PD}_{inter} : point defect interaction energy

Homogeneous stress: $\sigma_{ij} = \frac{1}{V}\frac{\partial E}{\partial \varepsilon_{ij}} = C_{ijkl}\varepsilon_{kl} - \frac{n^{PD}}{V}P_{ij}$

1) Conditions with **no stress** (experiments):

$\sigma_{ij} = 0$ ➔ $\varepsilon_{ij} = \frac{n^{PD}}{V}C^{-1}_{ijkl}P_{kl}$ (Vegard's law)

P_{ij} deduced from measured strain

2) Conditions with **no strain** (atomistic simulations):

$\varepsilon_{ij} = 0$ ➔ $\sigma_{ij} = -\frac{n^{PD}}{V}P_{ij}$

P_{ij} deduced from measured stress

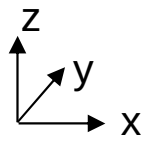
5. Carbon – Dislocation Interaction in Iron

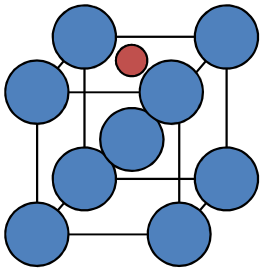
C atom in α iron:

interstitial in octahedral site with 3 variants: [100], [010], [001]

➔ modeled as a **point-force dipole**

[001] variant





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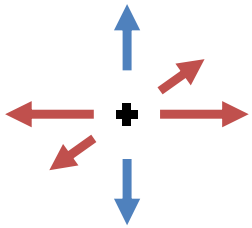


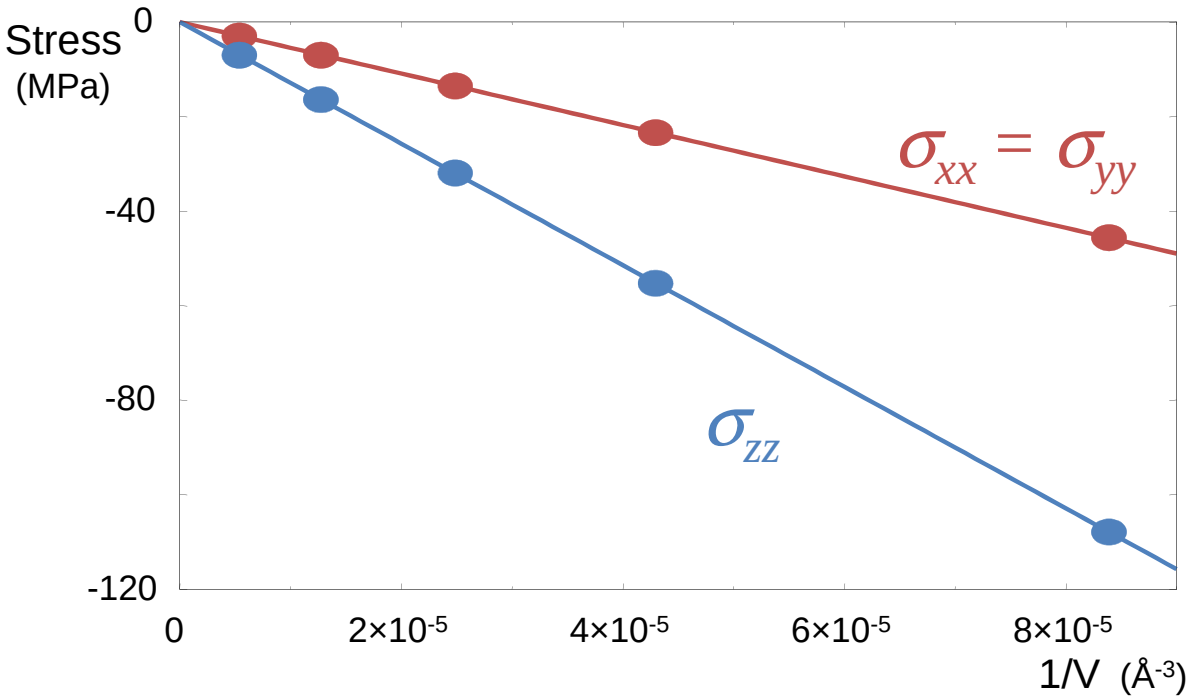
$$\left(P_{ij}\right) = \begin{pmatrix} P_x & 0 & 0 \\ 0 & P_y & 0 \\ 0 & 0 & P_z \end{pmatrix}$$

Atomic simulations:

- EAM potential[1,2]
- Atomic positions relaxed
- Periodicity vectors fixed: $\varepsilon_{ij} = 0$

➔ $$\sigma_{ij} = -\frac{1}{V} P_{ij}$$

$$\left(\sigma_{ij}\right) = -\frac{1}{V}\begin{pmatrix} P_x & 0 & 0 \\ 0 & P_x & 0 \\ 0 & 0 & P_z \end{pmatrix}$$



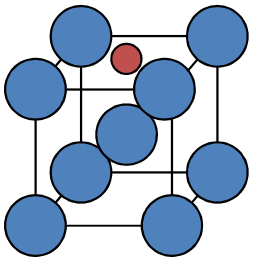
[1] M.I. Mendelev, S. Han, D.J. Srolovitz, G.J. Ackland, D.Y. Sun, M. Asta, *Philos. Mag.* **83**, 3977 (2003)

[2] C. Becquart, J. Raulot, G. Bencteux, C. Domain, M. Perez, S. Garruchet, & H. Nguyen, *Comp. Mater. Sci.* **40** (2007), 119.

5. Carbon – Dislocation Interaction in Iron

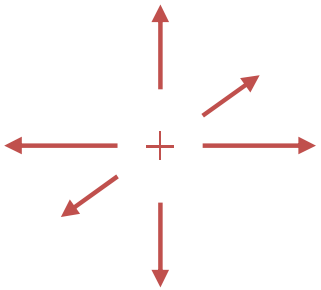
Atomistic simulations

- Empirical potential (EAM) for Fe-C alloys[1,2]
- Molecular statics (MS)
  - ➔ binding energies between
    - C atom in octahedral interstitial site
    - ½⟨111⟩{110} screw or edge dislocation



$$E^{bind} = E(dislo) + E(C) - E(dislo+C) - E(bcc)$$

Elasticity theory



$$E^{bind} = P_{ij}\varepsilon_{ij}^{d} = V\varepsilon_{ij}\sigma_{ij}^{d}$$

(model first proposed by Cochardt *et al.*[3])

ε_{ij}^{d} and $\sigma_{ij}^{d} = C_{ijkl}\varepsilon_{kl}^{d}$: strain and stress due to dislocation

calculated with
- isotropic elasticity
- anisotropic elasticity

When the point defect acts only as a dilatation center

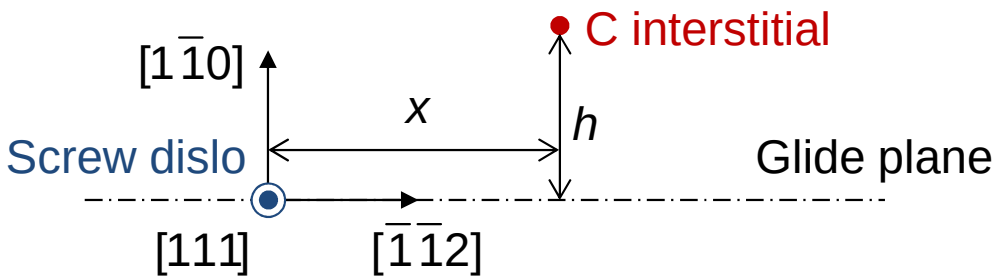
$E^{bind} = \delta\Omega \sum_i \sigma_{ii}^{d} / 3$ with $\delta\Omega = V \sum_i \varepsilon_{ii}$: point defect relaxation volume

("size interaction" model of Cottrell and Bilby[4])

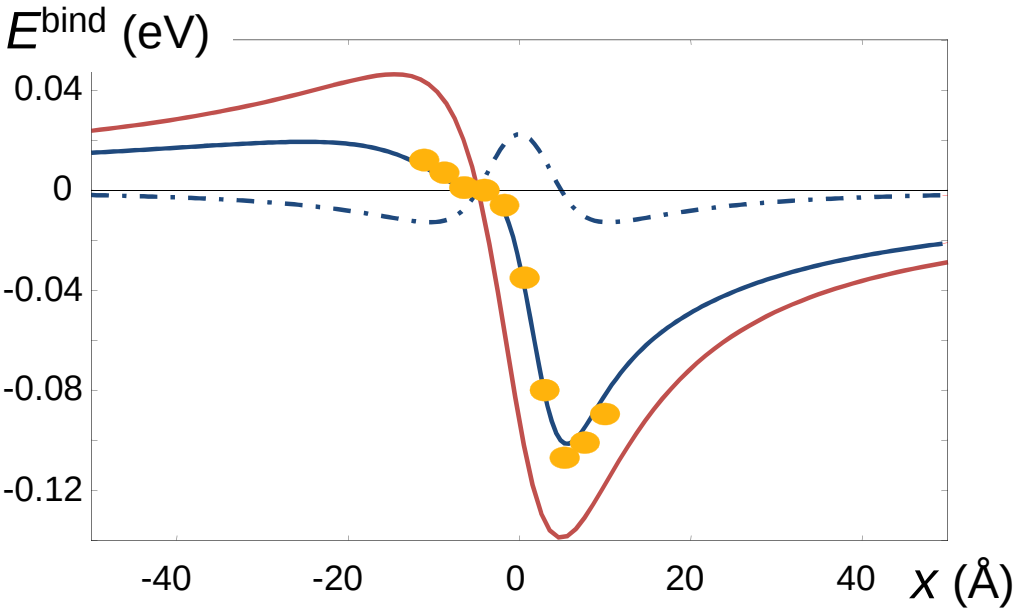
[1] M.I. Mendelev et al, *Philos. Mag.* **83**, 3977 (2003)
[2] C. Becquart,et al., *Comp. Mater. Sci.* **40**, 119 (2007)
[3] A. W. Cochardt, G. Schoek, and H. Wiedersich, *Acta Metall.* **3**, 533 (1955)
[4] A. H. Cottrell and B. A. Bilby, Proc. Phys. Soc. **A62**, 49 (1949)

5. Carbon – Dislocation Interaction in Iron

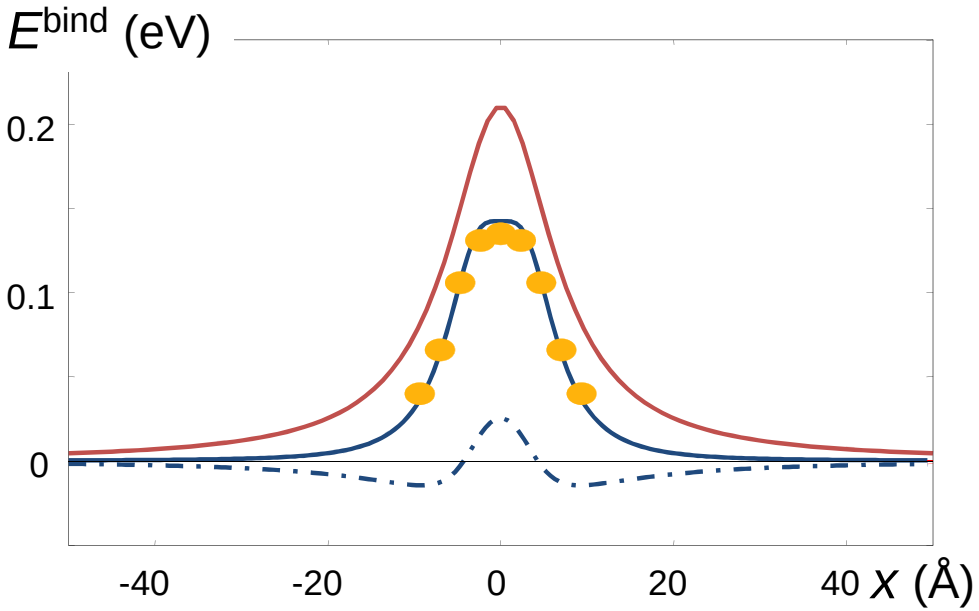
Screw dislocation



[100] variant – $h = 4d_{110}$



[001] variant – $h = 3.5d_{110}$



Anisotropic elasticity: all stress components

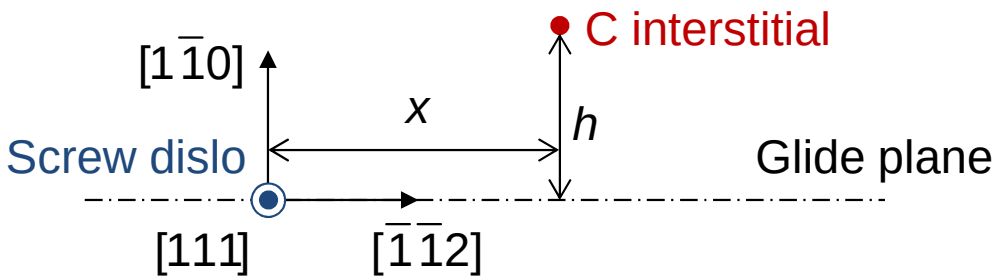
only pressure

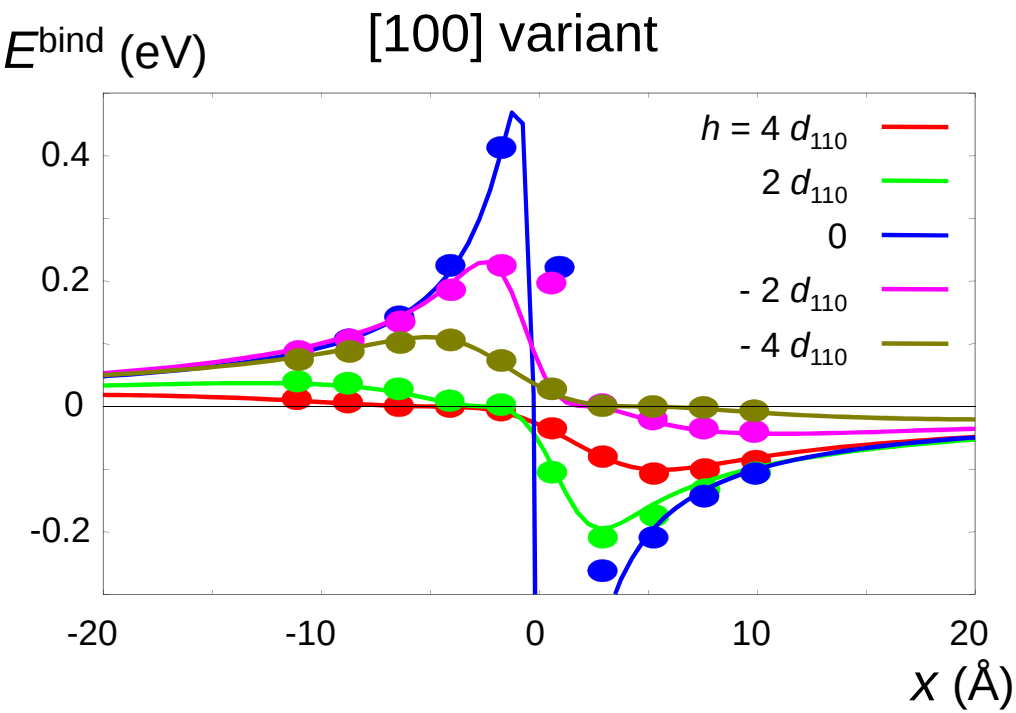
Isotropic elasticity: all stress components

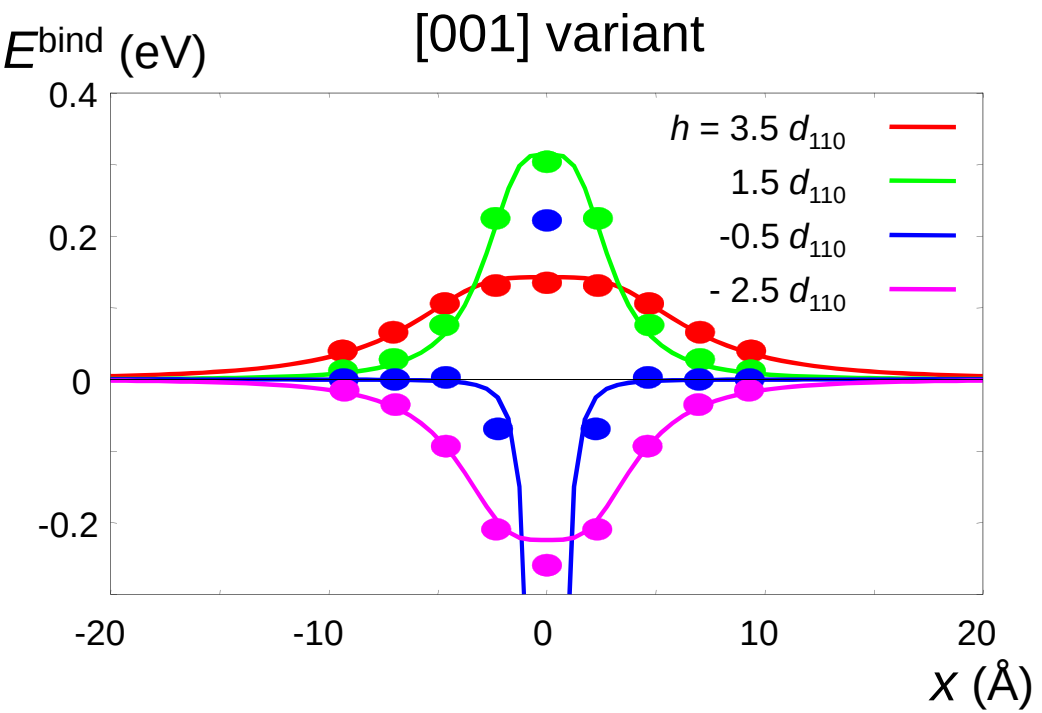
Atomic simulations

5. Carbon – Dislocation Interaction in Iron

Screw dislocation





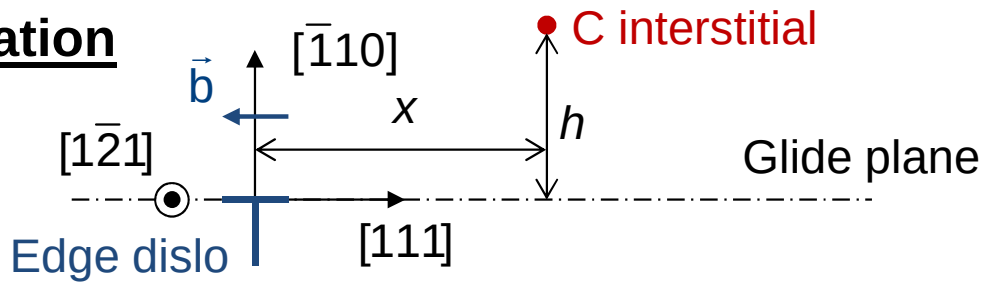


Anisotropic elasticity: all stress components

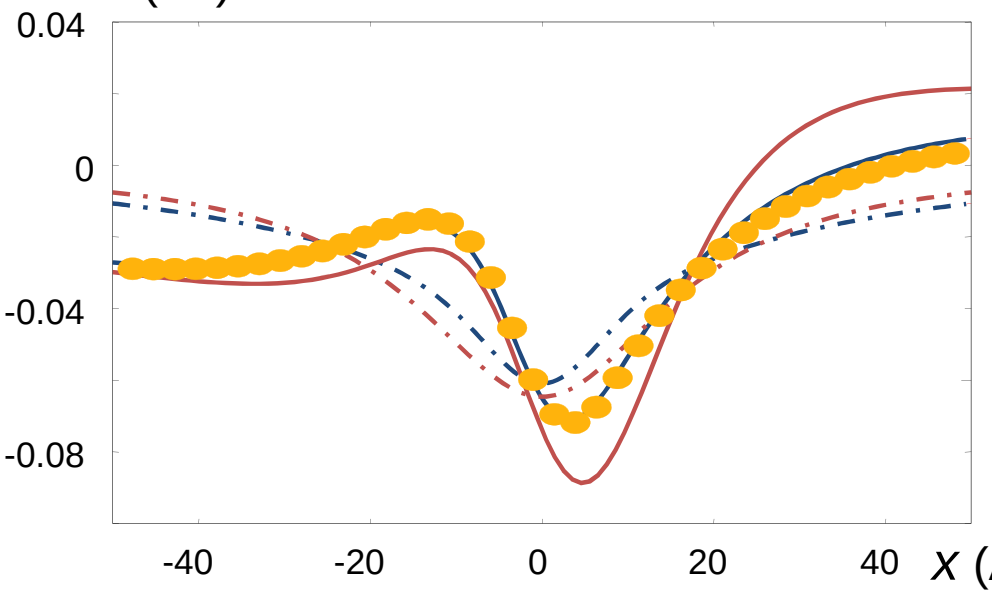
Atomic simulations

5. Carbon – Dislocation Interaction in Iron

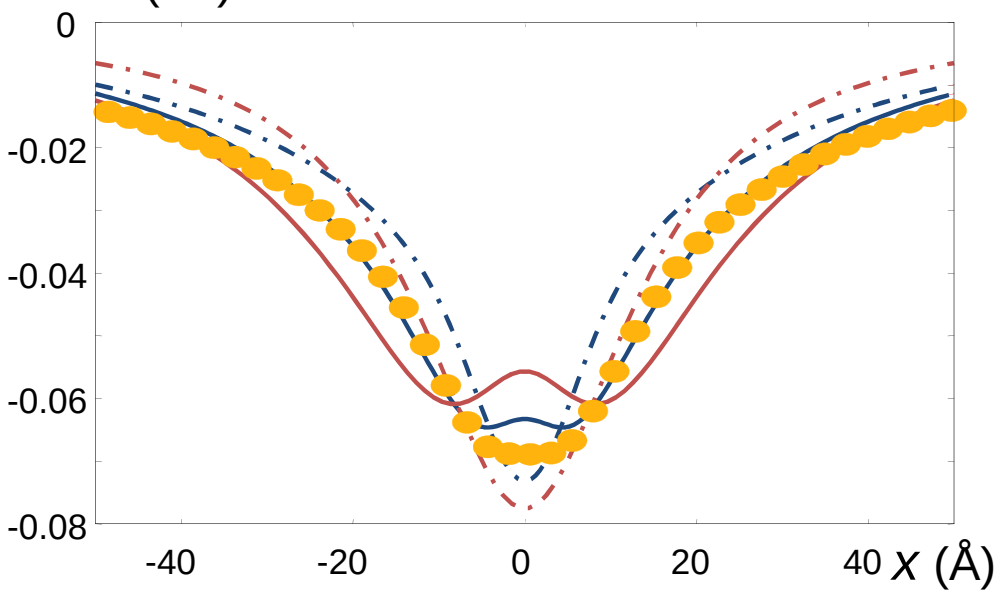
Edge dislocation



[100] variant – $h = -9d_{110}$



[010] variant – $h = -7.5d_{110}$



Anisotropic elasticity: all stress components

only pressure

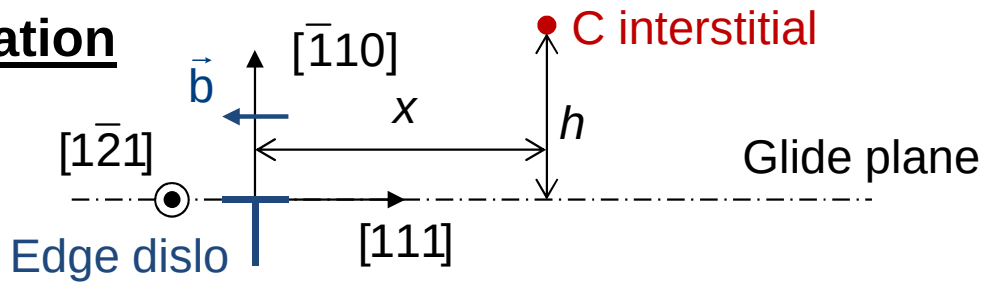
Isotropic elasticity: all stress components

only pressure

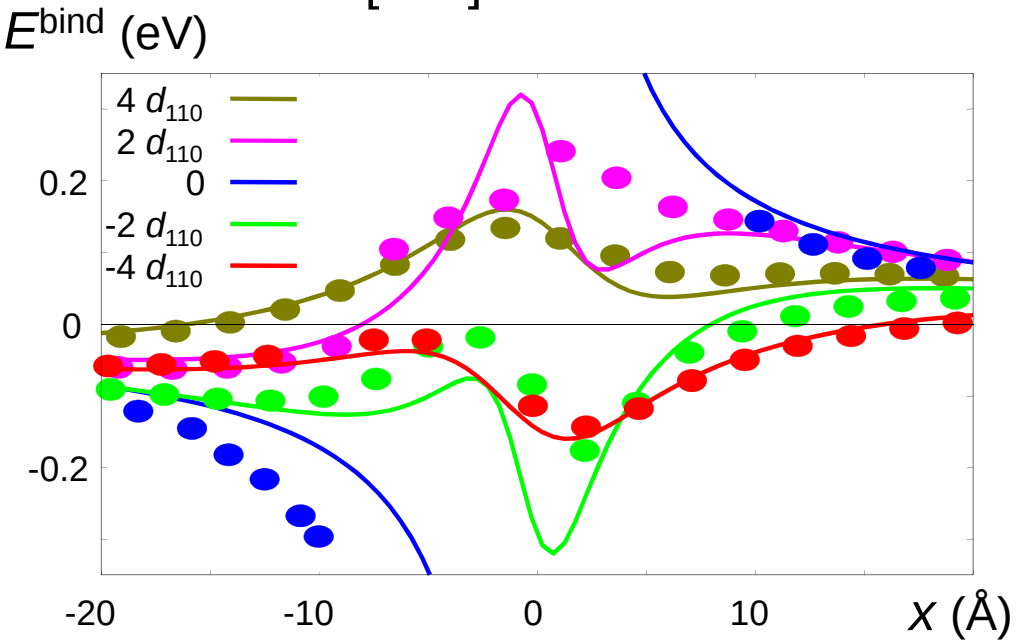
Atomic simulations

5. Carbon – Dislocation Interaction in Iron

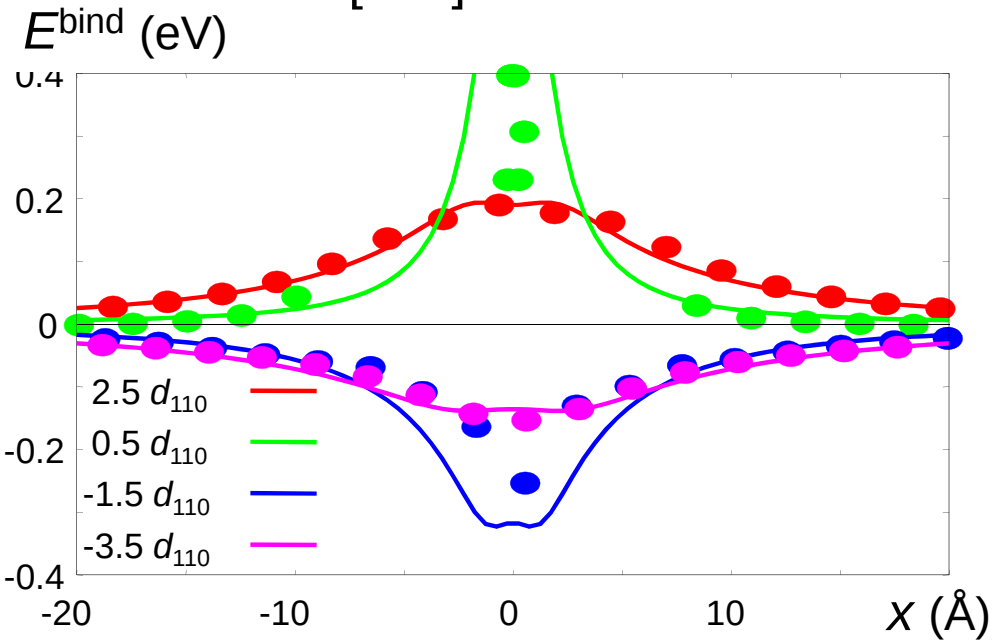
Edge dislocation



[100] variant



[010] variant



Anisotropic elasticity: all stress components

Atomic simulations

5. Carbon – Dislocation Interaction in Iron

Comparison atomic simulations / elasticity theory[1]

Quantitative agreement for $r > r_c$
when considering in elastic modeling

- dilatation and tetragonal distortion due to the C atom
- anisotropy

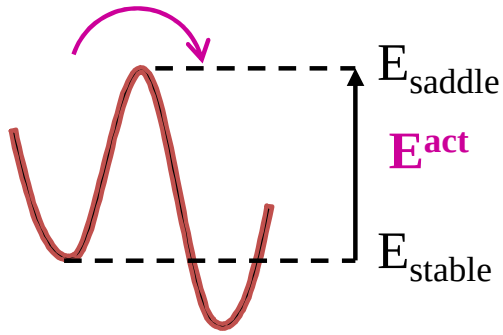
- screw: $r_c \sim 2$ Å
- edge: $r_c \sim 20$ Å

➔ elastic model can be used in mesoscale simulations (DD, AKMC, …)

Diffusion under stress[2]

Stress dependence of the activation energy
of the point-defect jump

$$E^{act} = E_{saddle} - E_{stable}$$
$$= E^0_{saddle} - E^0_{stable} - \left(P^{saddle}_{ij} - P^{stable}_{ij}\right)\varepsilon_{ij}$$



1 E. Clouet, S. Garruchet, H. Nguyen, M. Perez, and C.S. Becquart, *Acta Mater.* **56**, 3450 (2008)

2 R. Veiga, M. Perez, C. Becquart, E. Clouet and C. Domain, *Acta Mater.* **59**, 6963 (2011)

5. Carbon – Dislocation Interaction in Iron

Diffusion near the core

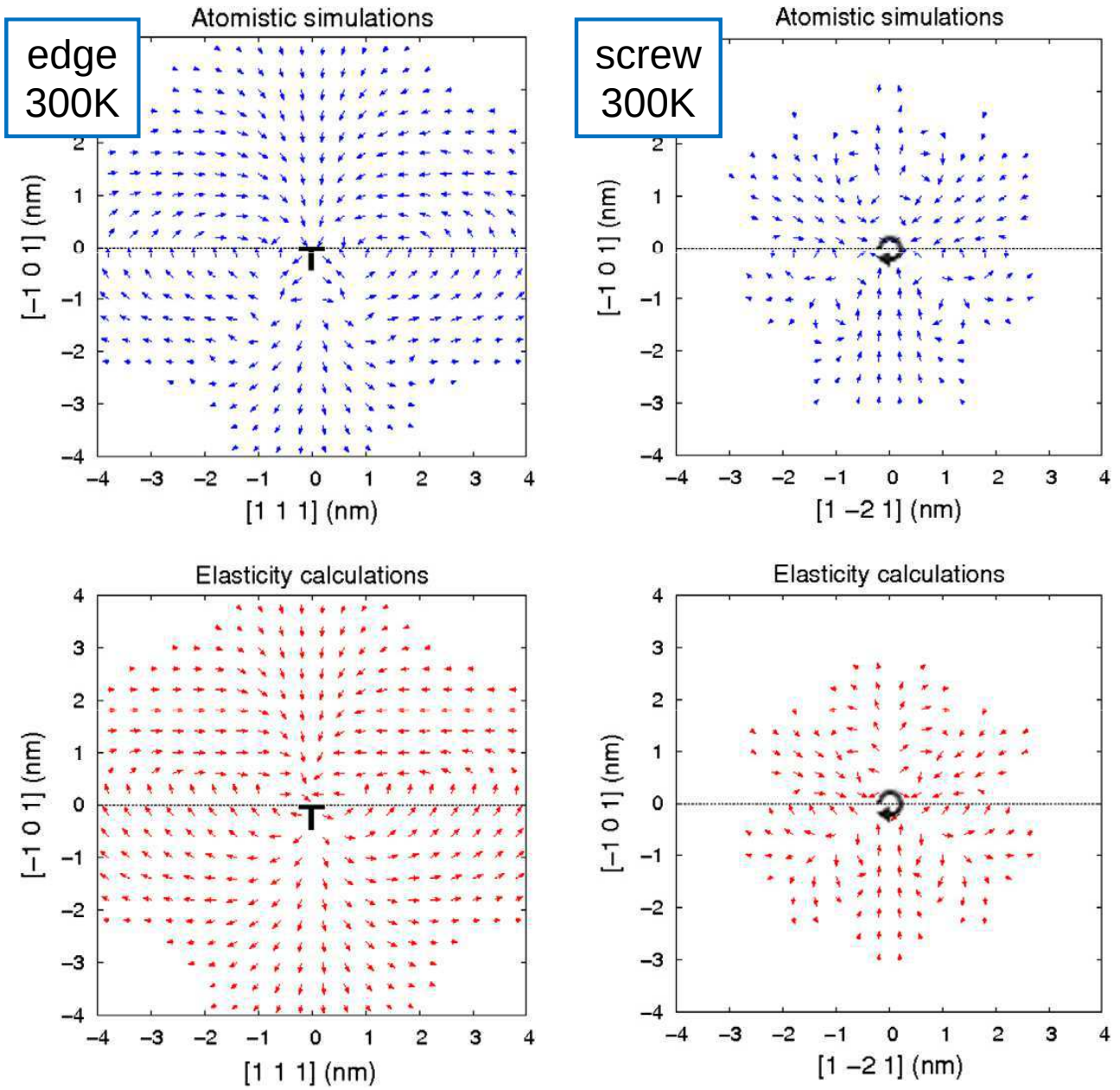
C diffusion bias induced by dislocation:

$$\left\langle \vec{d} \right\rangle = \sum_i P_{i\to j}\vec{\delta}_{i\to j}$$

$\vec{\delta}_{i\to j}$: jump vector

$P_{i\to j}$: jump probability
- EAM + NEB
- elasticity

➔ AKMC simulations



R. Veiga, M. Perez, C. Becquart, E. Clouet and C. Domain, Acta Mater. **59**, 6963 (2011)

6. Isolated Point-Defect in Ab Initio Calculations

Atomistic simulations: valuable tool to study **point defects**
(vacancies, self-interstitial atoms, solute, clusters, …)
➔ structure
➔ formation, migration, interaction energies

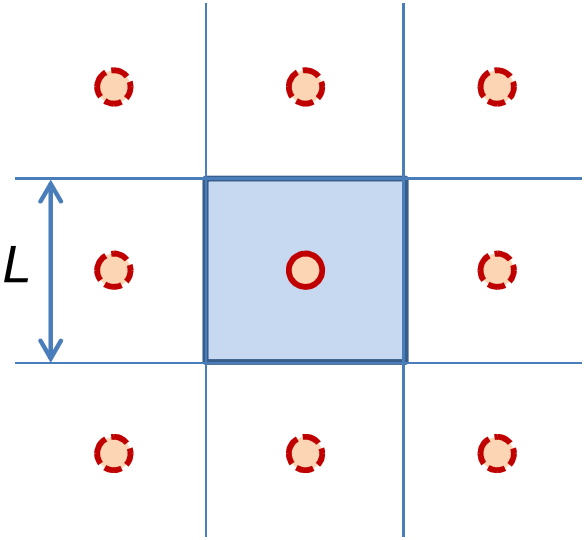
accuracy and transferability ↗ ↓

- empirical potentials
- ab initio calculations
  - DFT
  - hybrid functionals

↓ size of the system ↘

Point defects in a simulation cell
with **periodic boundary conditions**
➔ artifact due to interaction with periodic images

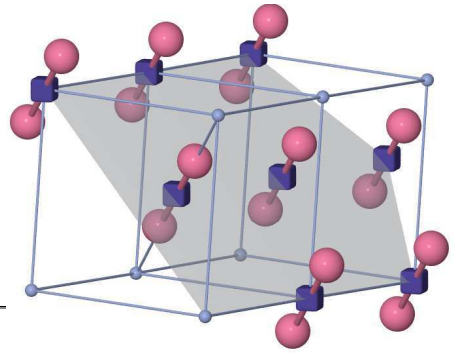
charged defect: Coulombian interaction ($E^{inter} \sim 1/L$)
neutral defect: **elastic interaction** ($E^{inter} \sim 1/L^3$)

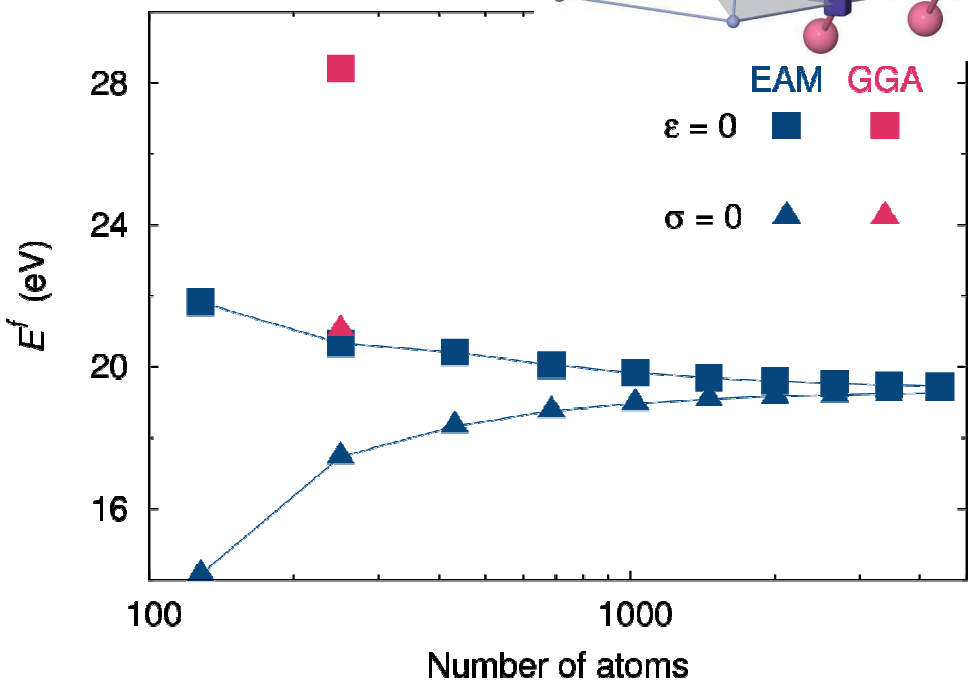


6. Isolated Point-Defect in Ab Initio Calculations

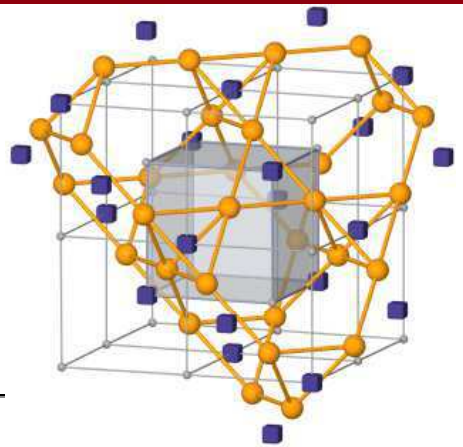
Self-interstitial clusters in bcc iron : Cluster containing 8 SIAs

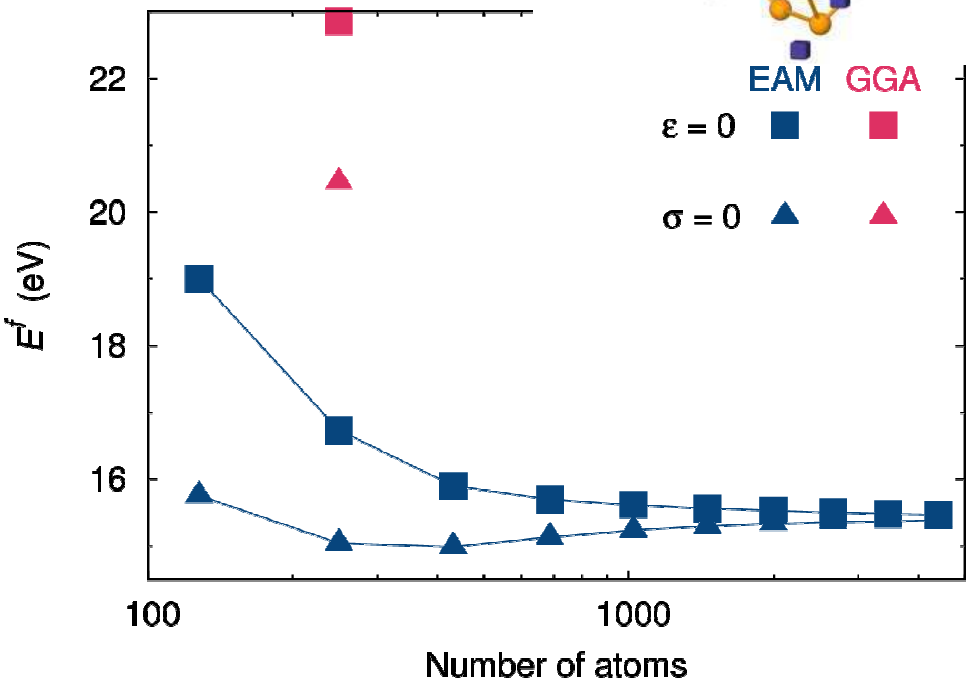
‹111› loop





C15 aggregate[1]





GGA ε=0 : ΔE = 5.6 eV
σ=0 : ΔE = 0.6 eV

1 M.-C. Marinica, F. Willaime, and J.-P. Crocombette, Phys. Rev. Lett. **108**, 025501 (2012).

6. Isolated Point-Defect in Ab Initio Calculations

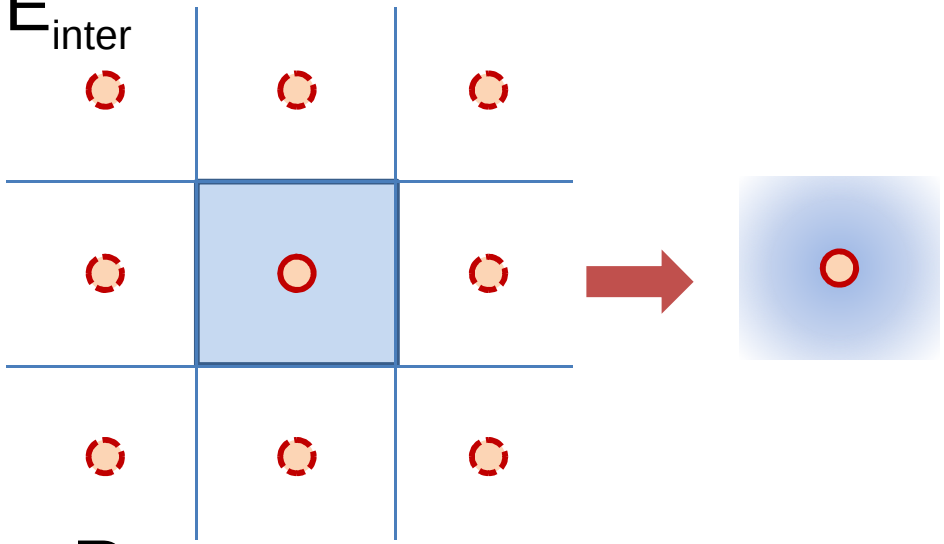
Atomistic simulations of point defects with **periodic boundary conditions**

→ $E^{PD}_{atomistic}$

Isolated point defect: $E^{PD}_{\infty} = E^{PD}_{atomistic} - 1/2\, E^{PBC}_{inter}$

Elasticity theory → E^{PBC}_{inter}

- withdraw artifact due to PBC
- consistency of ε=0 and σ=0 calculations



$$\varepsilon^{PBC}_{ij} = -\sum_{n,m,p}{}' G_{ik,jl}(\mathbf{R}_{nmp}) P_{kl} \quad \text{with} \quad \mathbf{R}_{nmp} = n\mathbf{a}_1 + m\mathbf{a}_2 + p\mathbf{a}_3$$

summation on periodic images

Inputs needed to evaluate interaction energy

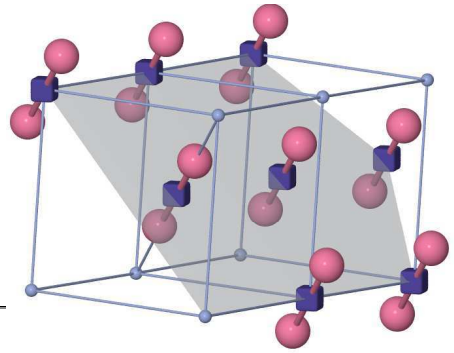
- **stress** / strain of the supercell containing the point defect: P_{ij}
- **elastic constants** of the perfect crystal: $G_{ik,jl}$

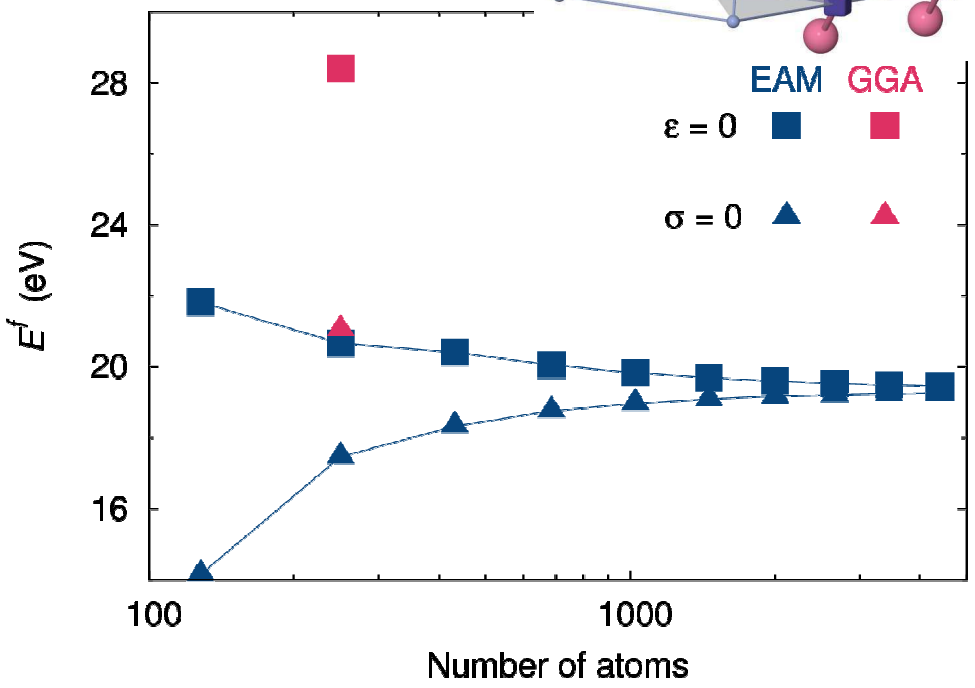
→ Fast and simple post-treatment

6. Isolated Point-Defect in Ab Initio Calculations

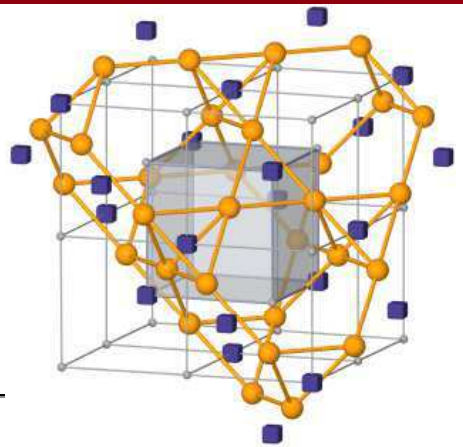
Self-interstitial clusters in bcc iron : Cluster containing 8 SIAs

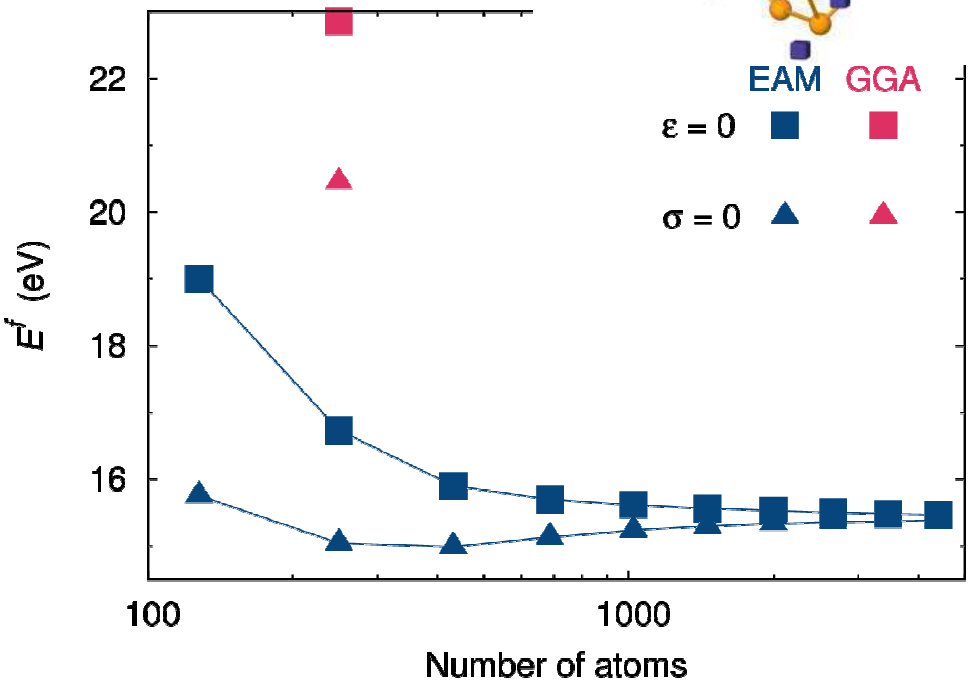
‹111› loop





C15 aggregate[1]





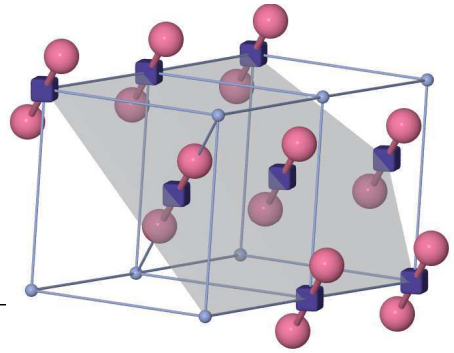
GGA ε=0 : ΔE = 5.6 eV
σ=0 : ΔE = 0.6 eV

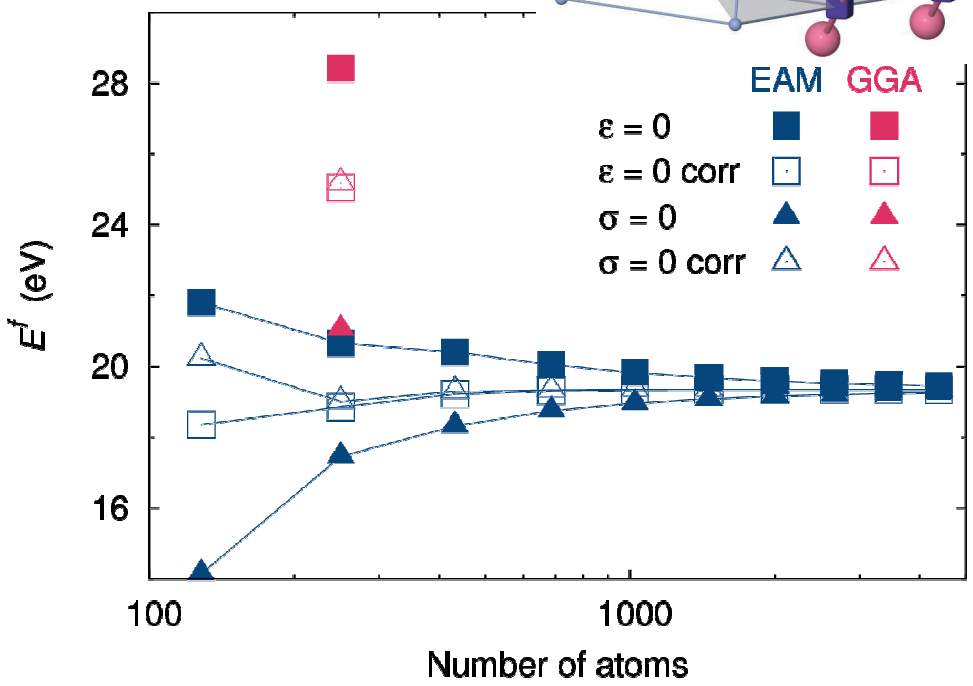
1 M.-C. Marinica, F. Willaime, and J.-P. Crocombette, Phys. Rev. Lett. **108**, 025501 (2012).

6. Isolated Point-Defect in Ab Initio Calculations

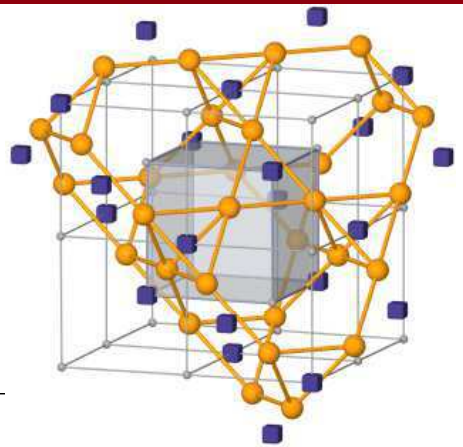
Cluster containing 8 self-interstitial atoms: formation energy

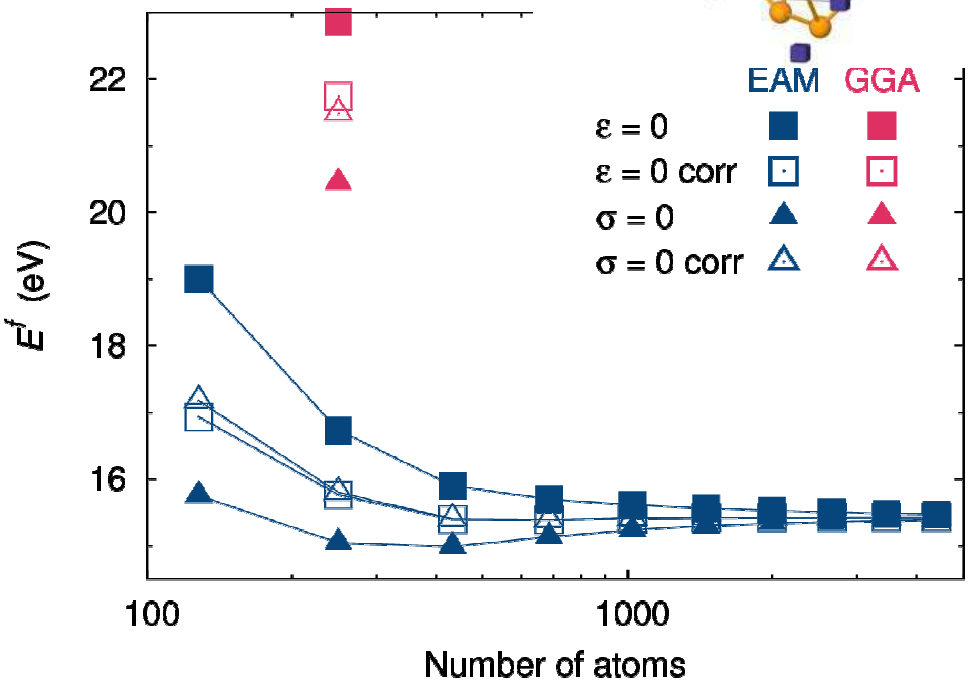
‹111› loop





C15 aggregate[1]





	Uncorrected	With elastic correction
GGA	ε=0 : ΔE = 5.6 eV	ε=0 : ΔE = 3.3 eV
	σ=0 : ΔE = 0.6 eV	σ=0 : ΔE = 3.7 eV

1 M.-C. Marinica, F. Willaime, and J.-P. Crocombette, Phys. Rev. Lett. **108**, 025501 (2012).

6. Isolated Point-Defect in Ab Initio Calculations

Neutral Vacancy in diamond Silicon

Si = **semi-conductors**: good description of the band gap needed

➔ simple DFT (LDA/GGA) fails

➔ RPA or hybrid functionals needed[1]

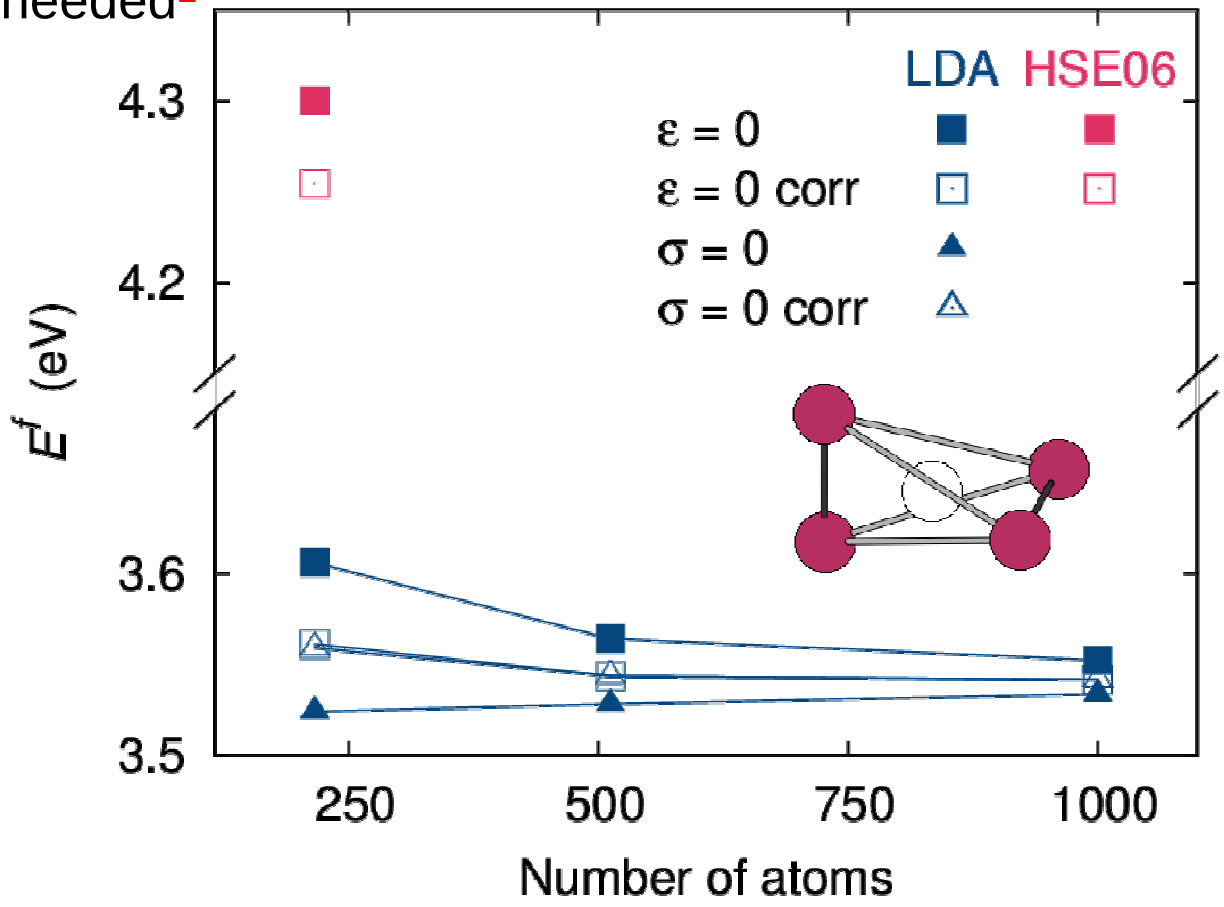
Vacancy: **Jahn-Teller distortion**

➔ long range elastic field

HSE06 hybrid functional

2x2x2 k-points mesh

➔ **E^f = 4.26 eV**



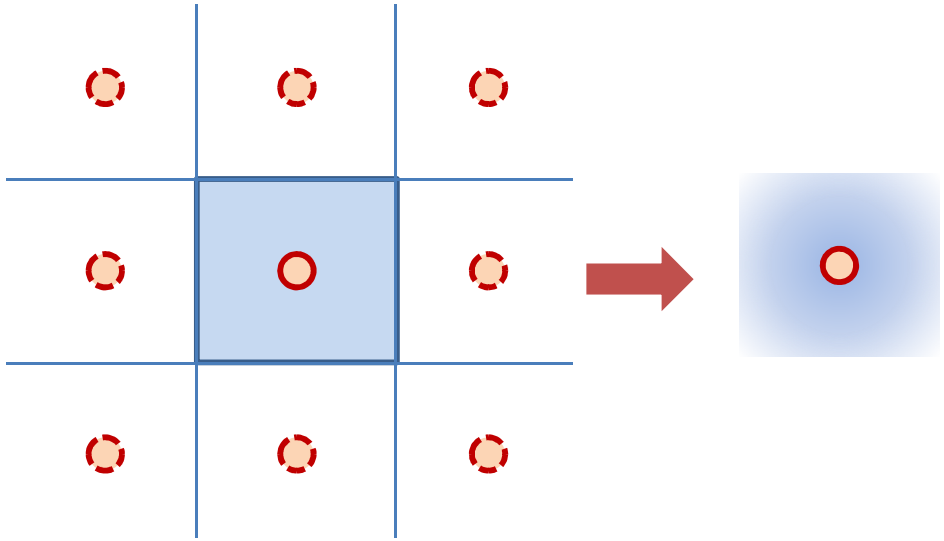
1 F. Bruneval, Phys. Rev. Lett. 108, 256403 (2012).

6. Isolated Point-Defect in Ab Initio Calculations

Conclusions

Isolated point defect:

$$E_{\infty}^{PD} = E_{atomistic}^{PD} - 1/2\, E_{inter}^{PBC}$$



Interaction energy evaluated
within anisotropic elasticity theory

Inputs:

- **elastic constants** of the perfect crystal
- **stress** / strain of the supercell containing the point defect

➔ Fast and simple post-treatment

(Fortran source code available as supplemental material♠)

Validation

- Interstitial clusters in bcc Fe
- Self-interstitial in hcp Zr (formation and migration)
- Neutral vacancy in silicon

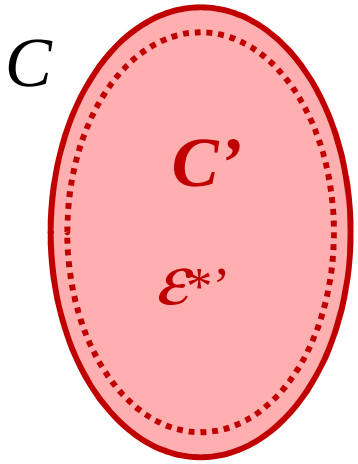
Perspective

Convergency could be improved by also correcting atomic forces
but the evaluation of $\partial^2 E / \partial X\, \partial \varepsilon$ is needed (no Hellmann-Feynamn theorem)

♠ C. Varvenne, F. Bruneval, M.-C. Marinica, and E. Clouet, Phys. Rev. B **in press** (2013).

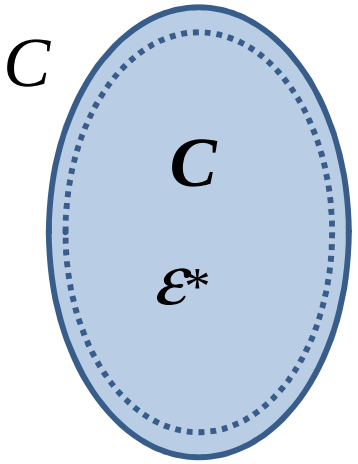
Eliispoidal inclusion

Eshelby **inhomogeneous** inclusion



Strain in the inclusion: $\varepsilon^{I'}$

equivalent **homogeneous** inclusion



Strain in the inclusion: $\varepsilon^{I} = S^{E}\,\varepsilon^{*}$

Displacement continuity at the interface: $\varepsilon^{I\,\prime} = \varepsilon^{I}$

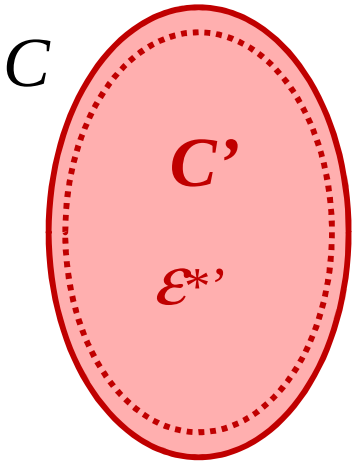
Stress continuity at the interface: $C'(\varepsilon^{I\,\prime} - \varepsilon^{*\,\prime}) = C(\varepsilon^{I} - \varepsilon^{*})$

$$\varepsilon^{*} = \left[(C' - C)S^{E} + C\right]^{-1} C'\varepsilon^{*\prime}$$

7. Inhomogeneity and polarizability

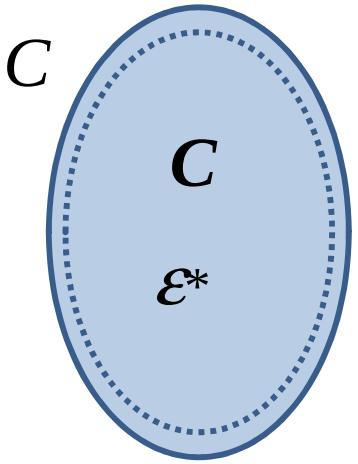
Ellipsoidal inclusion with an **applied strain**

Eshelby **inhomogeneous** inclusion



Strain in the inclusion: $\varepsilon^{I'} + \varepsilon^{A}$

equivalent **homogeneous** inclusion



Strain in the inclusion: $\varepsilon^{I} = S^{E}\,\varepsilon^{*} + \varepsilon^{A}$

Displacement continuity at the interface: $\varepsilon^{I\,\prime} + \varepsilon^{A} = \varepsilon^{I} + \varepsilon^{A}$

Stress continuity at the interface: $C'(\varepsilon^{I\,\prime} - \varepsilon^{*\,\prime} + \varepsilon^{A}) = C(\varepsilon^{I} - \varepsilon^{*} + \varepsilon^{A})$

$$\varepsilon^{*} = \left[(C' - C)S^{E} + C\right]^{-1}\left[C'\varepsilon^{*\prime} - (C' - C)\varepsilon^{A}\right]$$

➔ strain source depends on the applied strain

7. Inhomogeneity and polarizability

Point defect modeled in elasticity theory by an elastic dipole with an amplitude depending on the applied strain

first order:

$$P_{ij} = P_{ij}^{0} + \alpha_{ijkl}\varepsilon_{kl}$$

dipole (para-elasticity) — polarizability (dia-elasticity)

Elastic interaction with an applied strain

$$E^{inter} = -P_{ij}^{0}\varepsilon_{ij} - 1/2\,\alpha_{ijkl}\varepsilon_{ij}\varepsilon_{kl}$$

➔ dependence of the elastic constants with the concentration of point defects (solute atoms)

… two strain sources

$$E^{inter} = -P_{ij}^{0}\left(\varepsilon_{ij}^{(1)} + \varepsilon_{ij}^{(2)}\right) - \alpha_{ijkl}\varepsilon_{ij}^{(1)}\varepsilon_{kl}^{(2)} - 1/2\,\alpha_{ijkl}\left(\varepsilon_{ij}^{(1)}\varepsilon_{kl}^{(1)} + \varepsilon_{ij}^{(2)}\varepsilon_{kl}^{(2)}\right)$$

coupling (SIPA)

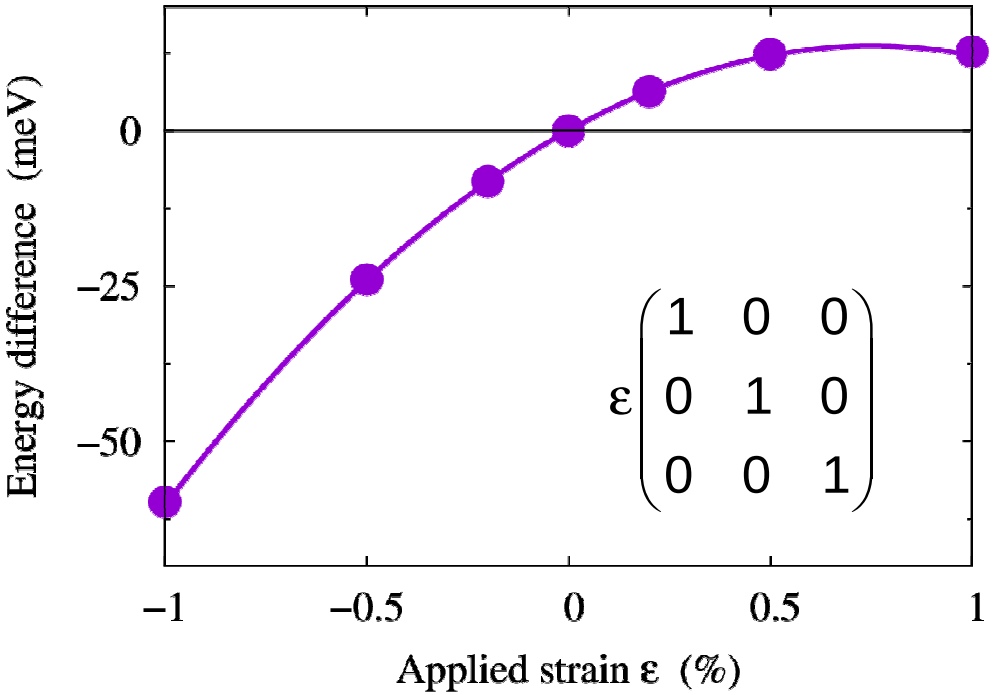
Under finite T, paraelastic contribution also leads to polarizability for a point defect with several variants

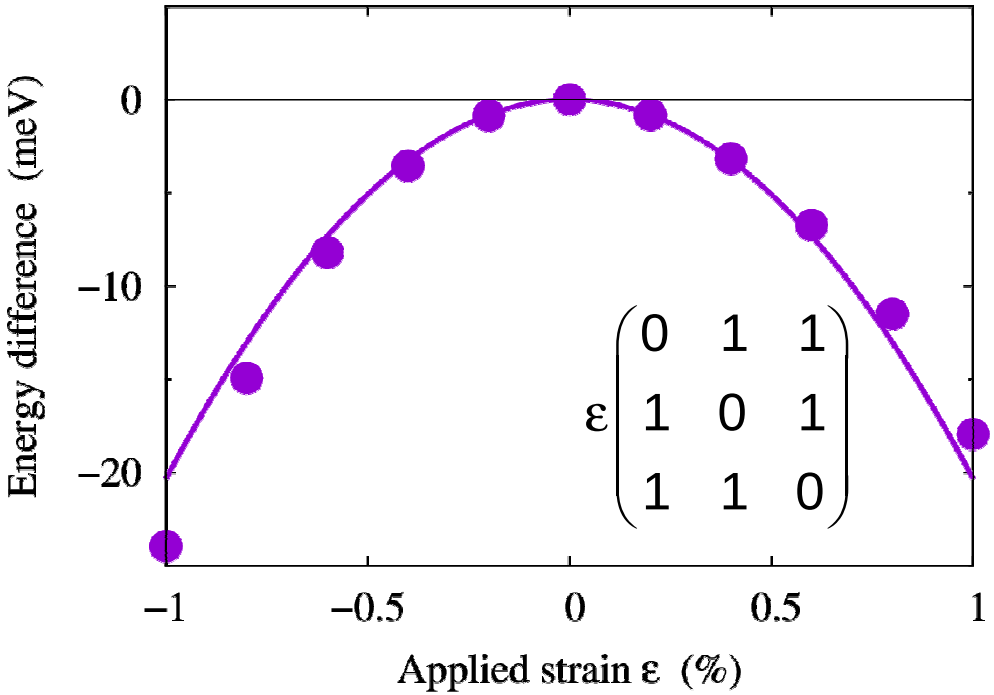
average dipole: $\left\langle P_{ij} \right\rangle = \sum_{n} \frac{\exp\left(-P_{kl}^{(n)}\varepsilon_{kl}\right)}{S} P_{ij}^{(n)}$ with $S = \sum_{m} \exp\left(-P_{kl}^{(m)}\varepsilon_{kl}\right)$

7. Inhomogeneity and polarizability

Vacancy in bcc iron : interaction with an applied strain

Simulation box 10x10x10 (2000 sites)
Marinica 2007 EAM potential





➔ elasticity can be used to model **variations with the applied strain** of the energies of defects (vacancies, self interstitials, solute, precipitates)

Morning's Conclusions

I. Elasticity Theory

1. Deformation of an elastic body
2. Stresses in an elastic body
3. Thermodynamics of deformation
4. Hooke's law
5. Equilibrium equation in homogeneous elasticity

II. Inclusions, Inhomogeneities and Point Defects

1. Spherical inclusion
2. Eshelby's inclusion
3. Inclusion and applied stress
4. Point defect
5. Carbon - dislocation interaction in iron
6. Isolated point-defect in ab initio calculations
7. Inhomogeneity and polarizability

III. Dislocations

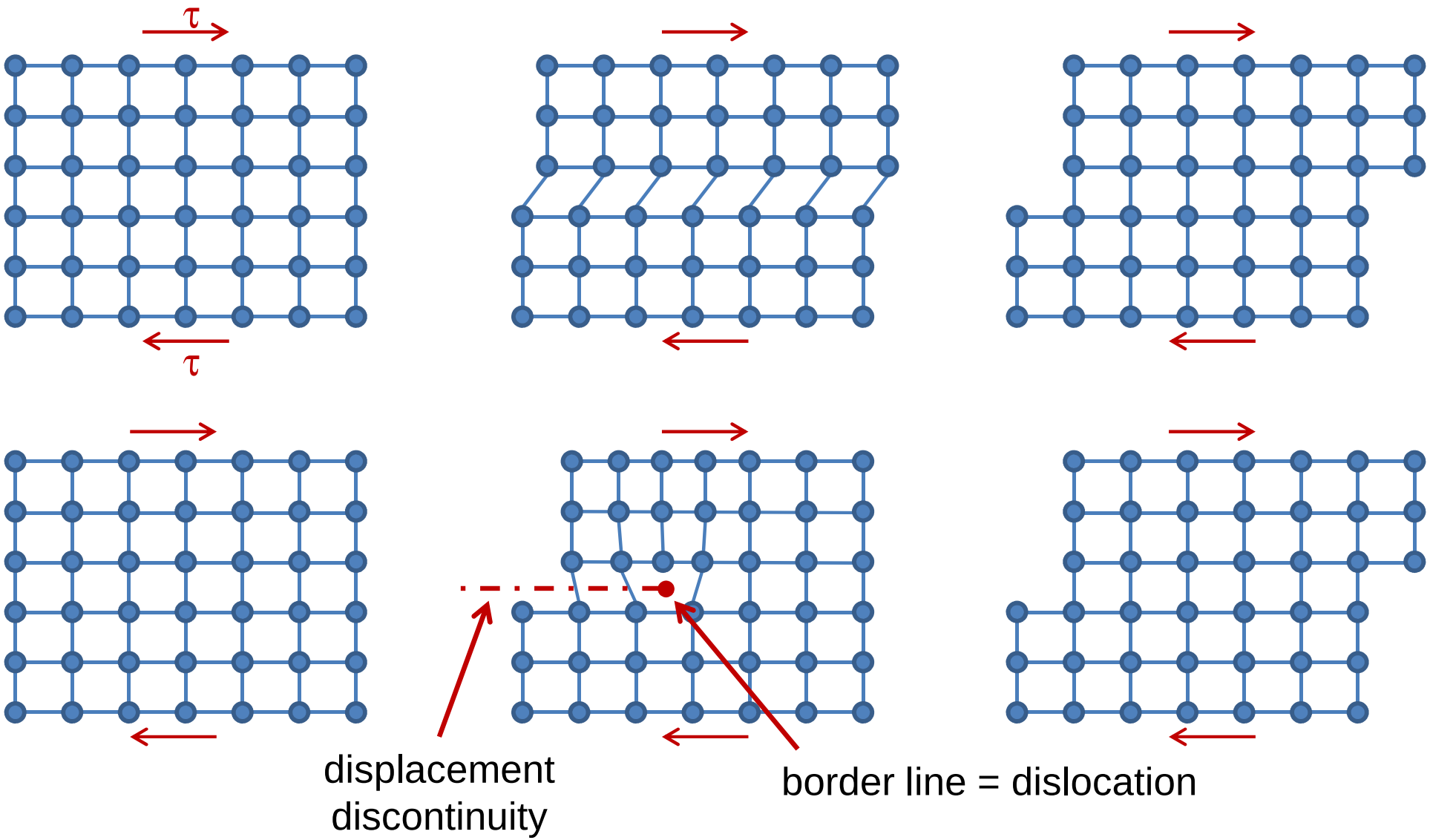
1. Dislocation: lattice defect
2. Elasticity theory of dislocations
3. Atomistic simulations
4. Dislocation dynamics
5. Crystal plasticity

References:

- D. J. Bacon, D. M. Barnett and R. O. Scattergood, Prog. Mater. Sci. **23**, 51 (1980).
- J.P. Hirth & J. Lothe, *Theory of dislocations* (1982)
- D. Hull and D. J. Bacon, *Introduction to Dislocations*, 5th edition (2011).
- V. V. Bulatov and W. Cai, *Computer Simulations of Dislocations* (2006).
- C. Weinberger, W. Cai and D. Barnett, *Elasticity of Microscopic Structures*, Standford Univ. lecture notes (2005).

1. Dislocation: lattice defect

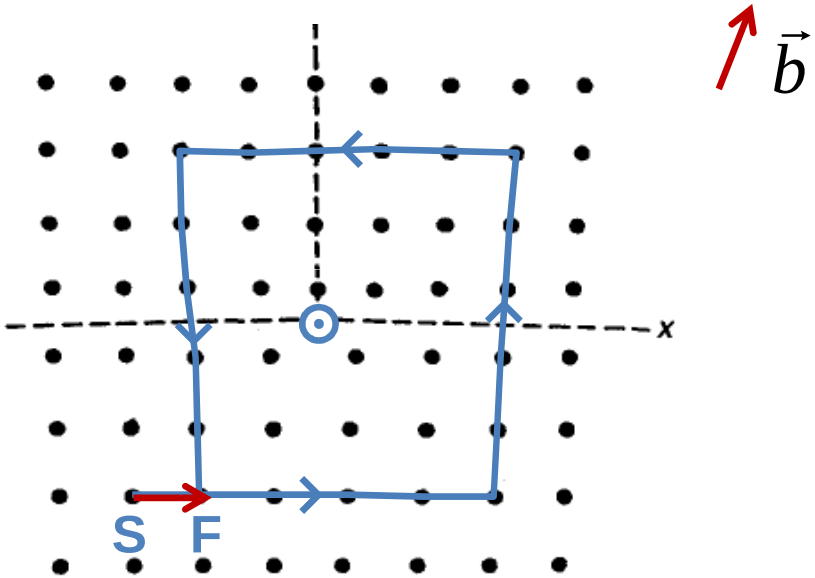
Crystal shear: homogeneous *vs* localized shear



Dislocation: frontier line of a surface of displacement discontinuity

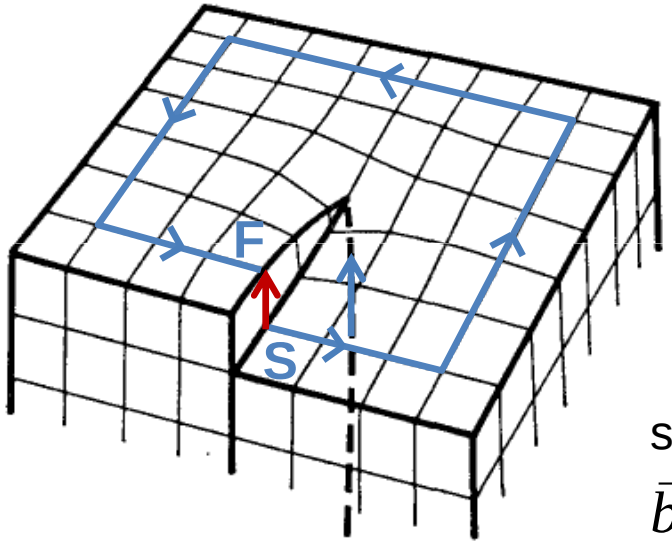
- line direction $\vec{l}$ (varying)
- Burgers vector $\vec{b} = \oint \mathrm{d}\vec{u}$ (conserved)

Linear crystal defect propagating the plastic strain



edge

$\vec{b} \perp \vec{\zeta}$



screw

$\vec{b} \parallel \vec{\zeta}$

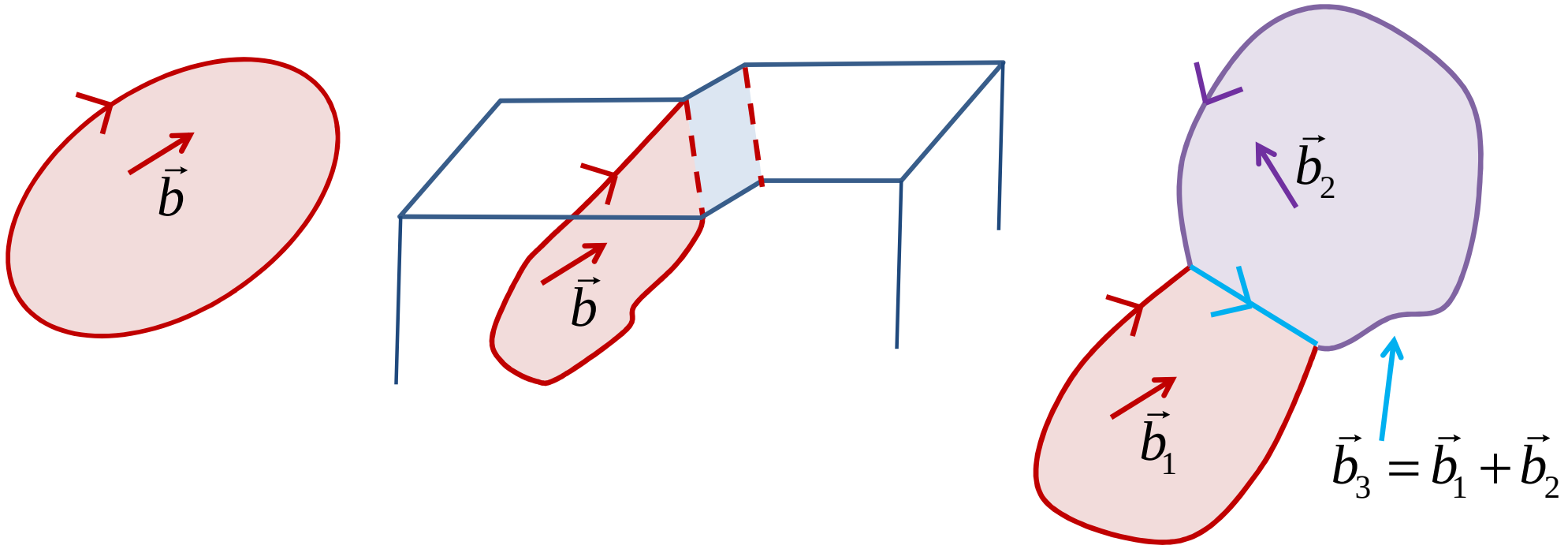
SF/RH convention

(see chap. 1 in Hirth and Lothe)

1. Dislocation: lattice defect

The displacement discontinuity needs to be **bound**

➔ close dislocation lines (loops)
or intersection with other defects (dislocations, surfaces)



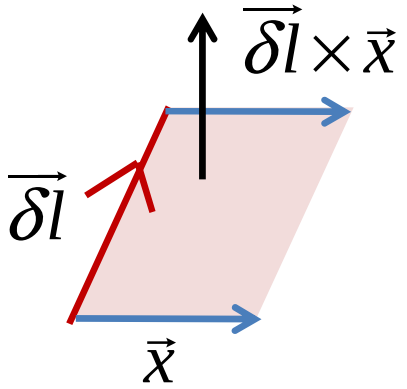
The Burgers vector needs to be a vector of the Bravais lattice
otherwise a stacking fault is generated (perfect *vs* partial dislocation)

1. Dislocation: lattice defect

When a dislocation segment advances, the corresponding surface area is displace by one Burgers vector.

The volume involved in the transformation is

$$\delta\Omega = (\overrightarrow{\delta l} \times \vec{x}) \cdot \vec{b} = (\vec{b} \times \overrightarrow{\delta l}) \cdot \vec{x}$$



Glide = conservative motion: $\delta\Omega = 0$

displacement needs to be orthogonal to line and Burgers vector

➔ Burgers vector and line direction belong to the glide plane

(screw dislocation: several glide planes)

Climb = non conservative motion: $\delta\Omega \neq 0$

displacement perpendicular to the glide plane

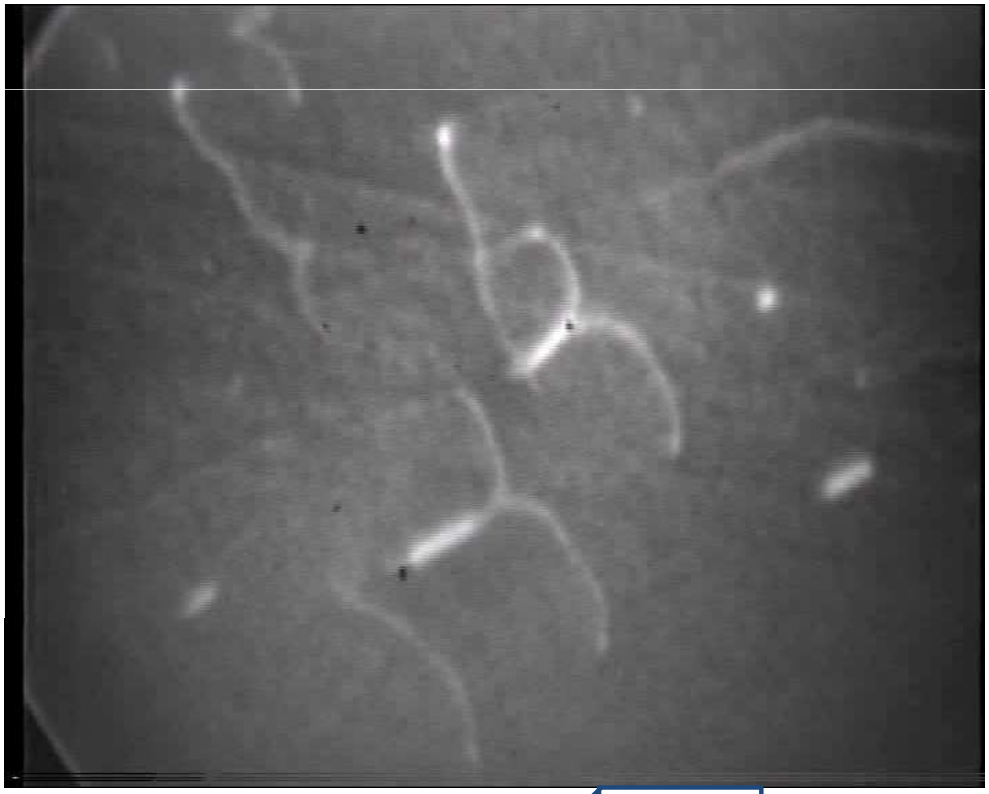
➔ diffusion needed

Dislocations in real life

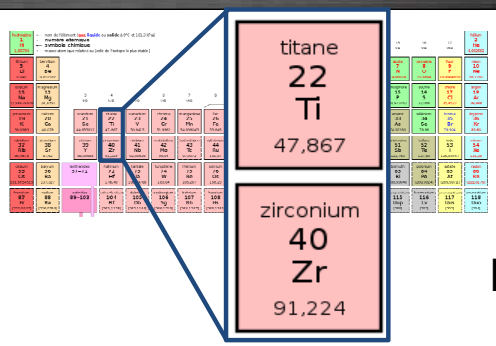
TEM in situ straining experiments

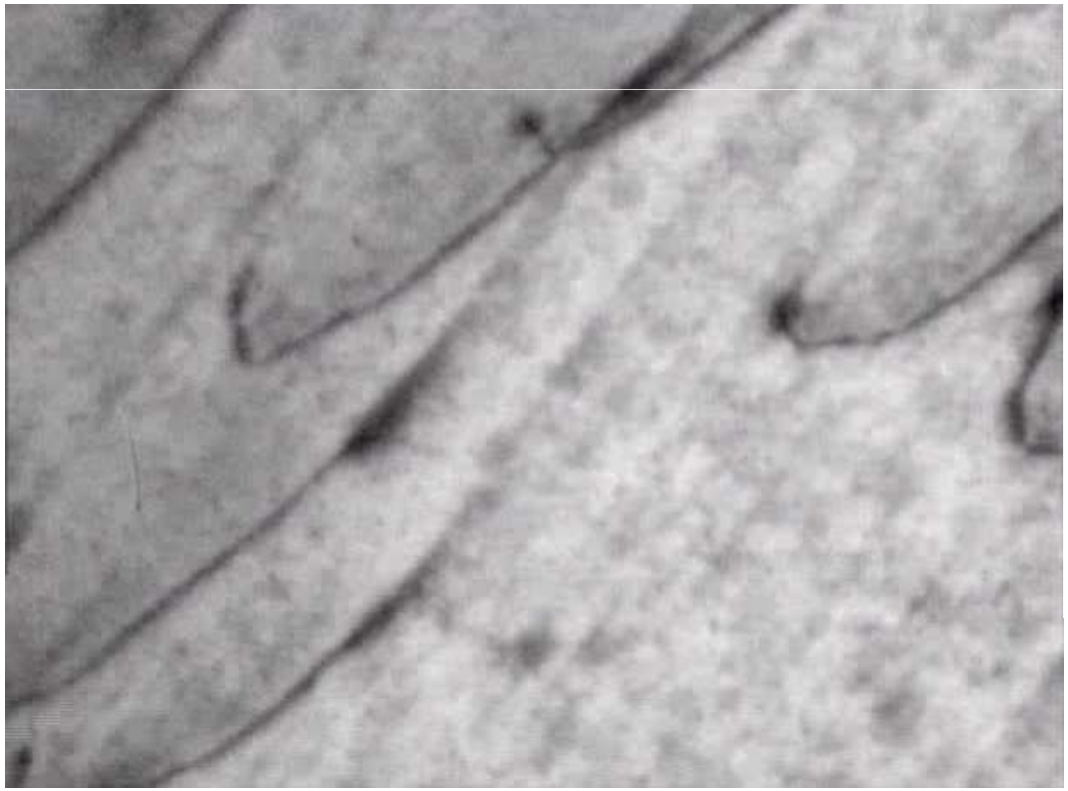
Daniel Caillard

CEMES



Ti @ 150 K

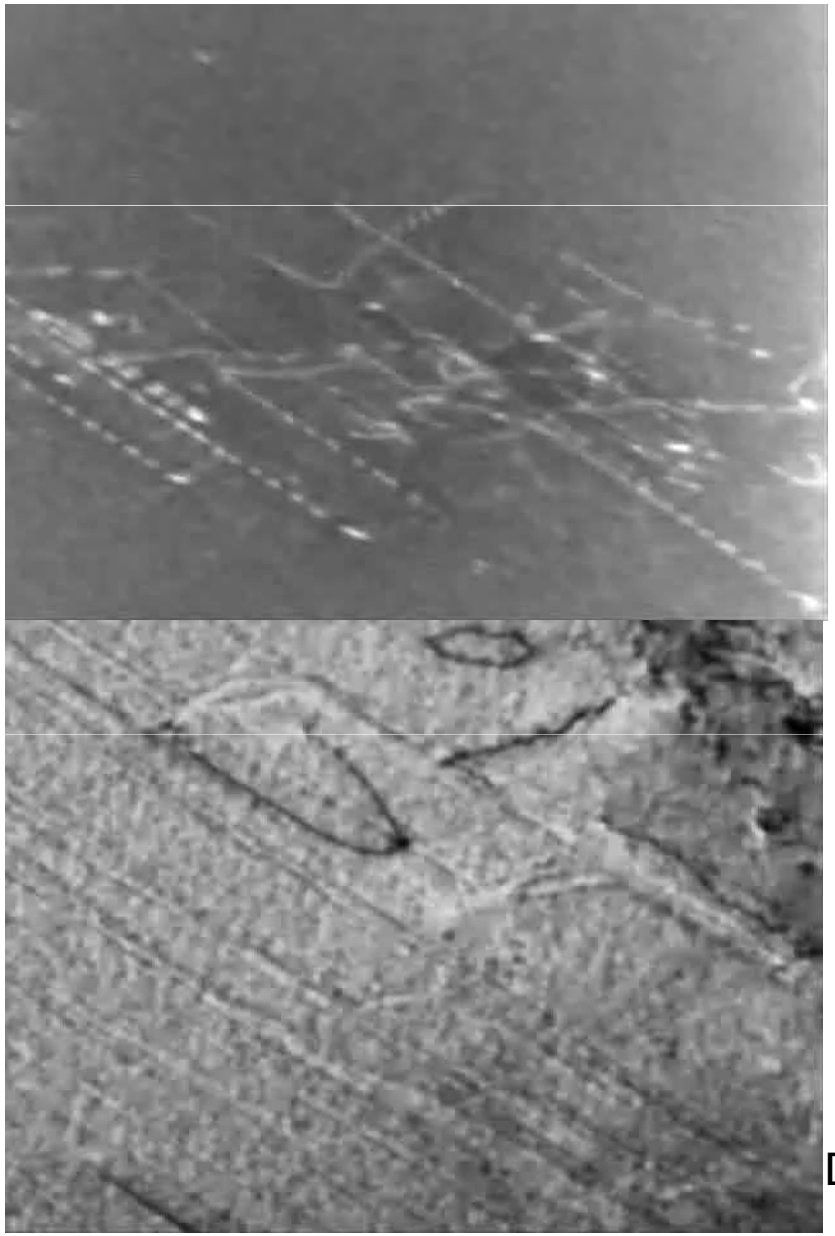




Zr @ 150 K

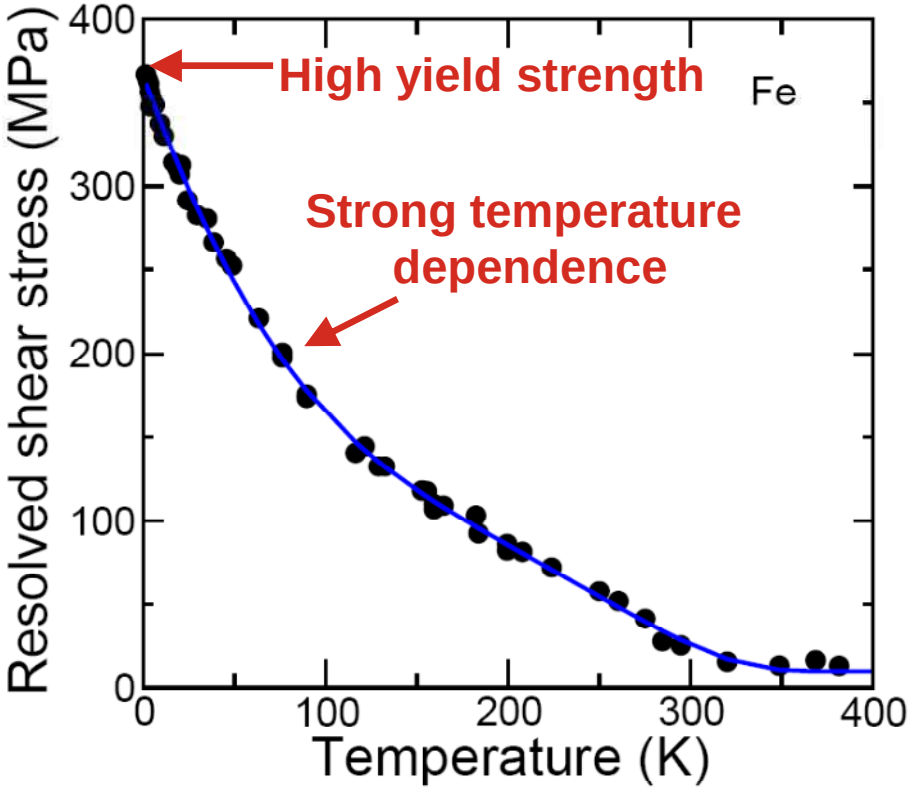
E. Clouet, D. Caillard, N. Chaari, F. Onimus and D. Rodney, Nature Materials in press (2015).

Dislocations in real life



Fe @ 120 K

Fe @ ambiant T

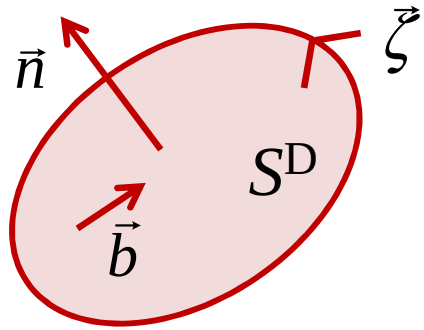


D. Brunner and J. Diehl, Phys. Stat. Sol. A **160**, 355 (1997).
D. Caillard, Acta Mater. **58**, 3493; 3504 (2010).

Linear elasticity theory

$$C_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l} + f_i = 0 \qquad \sigma_{ij} = C_{ijkl}\varepsilon_{kl} \quad \text{and} \quad \varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Dislocation definition: $\vec{b} = \oint \mathrm{d}\vec{u}$



Elastic field created by a dislocation loop in an infinite body

$$u_i(\vec{x}) = C_{jklm} b_m \int_{S^{\mathrm{D}}} n_l G_{ij,k}(\vec{x} - \vec{x}')\mathrm{d}S' \qquad \text{(Volterra's formula)}$$

$$\sigma_{ij}(\vec{x}) = C_{ijkl} \oint_{L^{\mathrm{D}}} \epsilon_{lnh} C_{pqmn} b_m \zeta_h(\vec{x}') G_{kp,q}(\vec{x} - \vec{x}')\mathrm{d}l' \qquad \text{(Mura's formula)}$$

with ζ_h unit vector along the line

displacement: surface integral ➔ depends on history
stress: line integral ➔ state variable

computer implementation of stress calculations: DD simulations

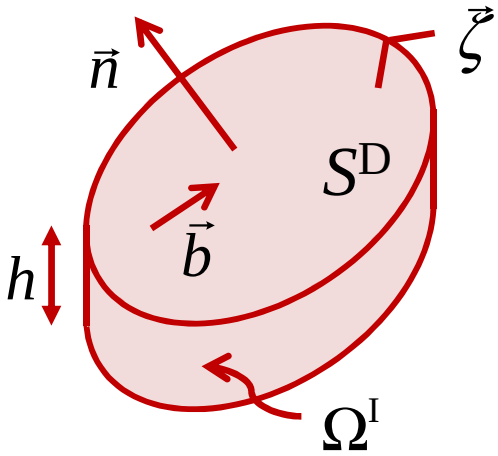
divergence close to the dislocation line: $\ln(r)$ for displacement

$1/r$ for stress

Elastic field created by a dislocation loop in an infinite body

$$u_i(\vec{x}) = C_{jklm} b_m \int_{S^D} n_l G_{ij,k}(\vec{x} - \vec{x}') \mathrm{d}S'$$

$$= \lim_{h \to 0} \left[C_{jklm} \int_{\Omega^I} \varepsilon^*_{ml} G_{ij,k}(\vec{x} - \vec{x}') \mathrm{d}V' \right]$$



➔ Dislocation loop equivalent to an **Eshelby inclusion**

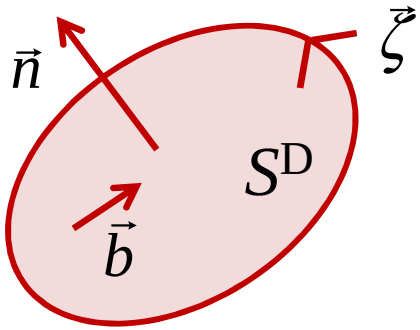
- volume $\Omega^I = hS$
- eigenstrain $\varepsilon^*_{ml} = -\dfrac{b_m n_l}{h}$

2. Elasticity theory of dislocations

Elastic field created by a dislocation loop in an infinite body
far from the loop

$$u_i(\vec{x}) = C_{jklm} b_m \int_{S^D} n_l G_{ij,k}(\vec{x} - \vec{x}') \mathrm{d}S'$$
$$= C_{jklm} b_m S_l G_{ij,k}(\vec{x})$$

$$\rightarrow \quad u_i(\vec{x}) \propto \frac{1}{\|\vec{x}\|^2}$$



$$\sigma_{pq}(\vec{x}) = C_{pqin} C_{jklm} b_m S_l G_{ij,kn}(\vec{x}) \quad \rightarrow \quad \sigma_{ij}(\vec{x}) \propto \frac{1}{\|\vec{x}\|^3}$$

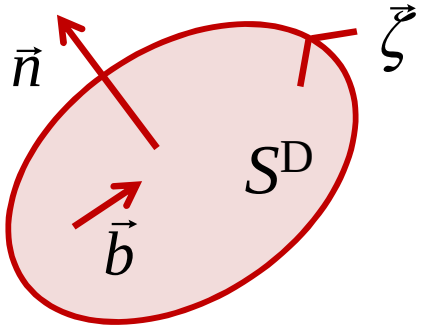
Infinitesimal dislocation loop can model a **point defect**
elastic dipole

$$P_{ij} = -C_{ijkl} b_k S_l^D$$

Interaction with an applied stress

using Gauss theorem

$$E^{\text{inter}} = \int_V \sigma_{ij}^{\text{A}} \varepsilon_{ij}^{\text{D}} \mathrm{d}V = \int_V \sigma_{ij}^{\text{A}} \frac{\partial u_i^{\text{D}}}{\partial x_j} \mathrm{d}V$$



$$= \int_V \frac{\partial}{\partial x_j}\left(\sigma_{ij}^{\text{A}} u_i^{\text{D}}\right)\mathrm{d}V - \int_V \frac{\partial \sigma_{ij}^{\text{A}}}{\partial x_j} u_i^{\text{D}} \mathrm{d}V$$

$$= \int_{S^{\text{D+}} \cup S^{\text{D-}}} \sigma_{ij}^{\text{A}} u_i^{\text{D}} \mathrm{d}S_j$$

= 0 (equilibrium)

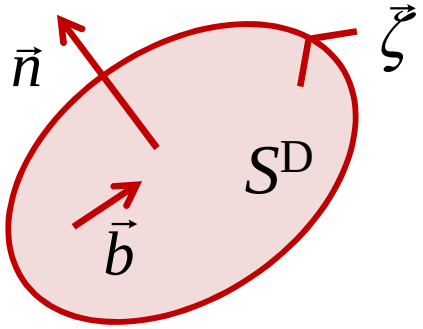
$$= \int_{S^{\text{D}}} \sigma_{ij}^{\text{A}} b_i \mathrm{d}S_j$$

using analogy with Eshelby inclusion

$$E^{\text{inter}} = -\int_{\Omega^{\text{I}}} C_{ijkl} \varepsilon_{ij}^{*}(\vec{x}) \varepsilon_{kl}^{\text{A}}(\vec{x}) \mathrm{d}V \quad \text{with} \quad \Omega^{\text{I}} = hS^{\text{D}} \quad \text{and} \quad \varepsilon_{ml}^{*} = -\frac{b_m n_l}{h}$$

➔ $$\boxed{E^{\text{inter}} = \int_{S^{\text{D}}} \sigma_{ij}^{\text{A}} b_i \mathrm{d}S_j}$$

Interaction with an applied stress



$$E^{\mathrm{inter}} = \int_{S^{\mathrm{D}}} \sigma_{ij}^{\mathrm{A}} b_i \mathrm{d}S_j$$

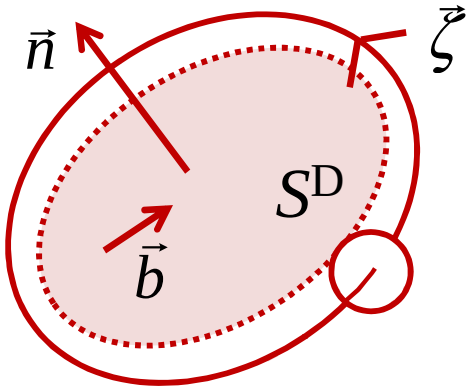
Energy variation δE when the dislocation sweeps an infinitesimal surface area δS^{D}

➔ Peach Koehler force

$$\vec{F}^{\mathrm{PK}} = \left(\boldsymbol{\sigma}^{\mathrm{A}} \vec{b}\right) \times \vec{\zeta}$$

Dislocation self energy

$$E^{\mathrm{D}} = \frac{1}{2}\int_V \sigma_{ij}^{\mathrm{D}} \varepsilon_{ij}^{\mathrm{D}} \mathrm{d}V$$



➔ needs to introduce a cutoff distance, **core radius** r_{c}, to avoid divergence in the core

inside the core region: **core energy**

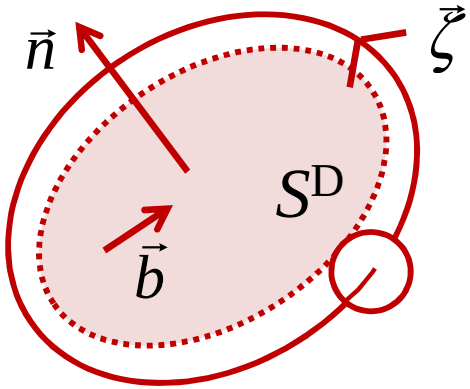
outside: elastic energy
can be obtained by a double line integral[1]
+ tractions on the core cylinder[2]

➔ other solution = spreading of the Dirac peak defining the density of Burgers vector: Peierls Nabarro, standard core[3], non singular theory[4]

➔ the self energy induces a **self stress**

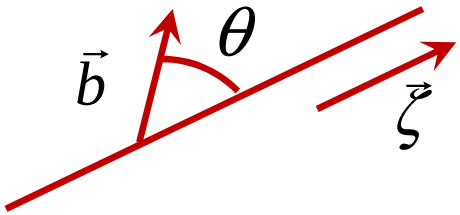
1. J. Lothe, Philos. Mag. A 46, 177 (1982).
2. E. Clouet, Philos. Mag. 89, 1565 (2009).
3. J. Lothe, Dislocations in Continuous Elastic Media, 187 (1992).
4. W. Cai, A. Arsenlis, C. R. Weinberger and V. V. Bulatov, J. Mech. Phys. Solids 54, 561 (2006).

Dislocation self energy: line tension approximation



$$E^{\mathrm{D}} = \frac{1}{2}\int_V \sigma_{ij}^{\mathrm{D}} \varepsilon_{ij}^{\mathrm{D}} \mathrm{d}V$$

$$E^{\mathrm{D}} = \int_{L^{\mathrm{D}}} E^{\infty}(\theta)\mathrm{d}l$$



with $E^{\infty}(\theta) = \frac{1}{2}K(\theta)b^2 \log\left(\frac{R}{r_c}\right)$ energy of an infinite straight dislocation of same character θ

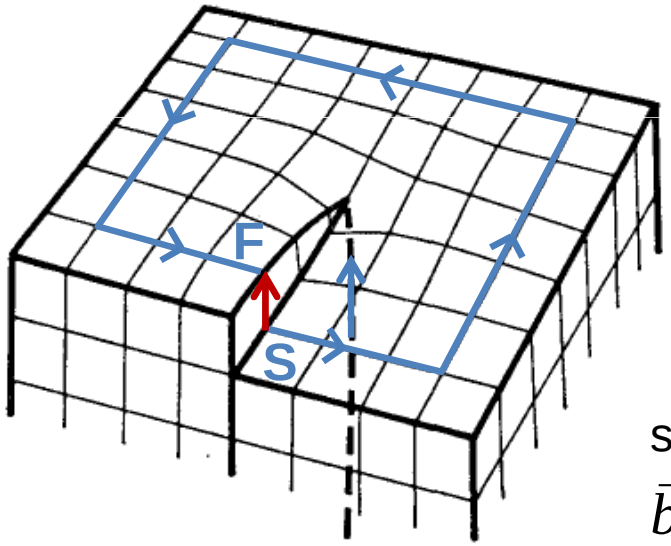
R characteristic size of the loop

➔ $E^{\mathrm{D}} \propto R[\log(R) + cste]$

Self stress $\tau = -\frac{\Gamma}{\rho b}$ line tension $\Gamma = E(\theta) + \frac{\partial^2 E(\theta)}{\partial \theta^2}$

dislocation curvature radius ρ

Infinite straight dislocation: screw in isotropic elasticity



screw
$\vec{b} \parallel \vec{\zeta}$

cylindrical symmetry

$$\vec{u}(\rho) = b\frac{\theta}{2\pi}\vec{e}_z \quad \propto \log(\rho)$$

$$\begin{cases} \sigma_{\theta z} = \dfrac{\mu b}{2\pi\rho} & \propto \dfrac{1}{\rho} \\ \sigma_{\rho\rho} = \sigma_{\theta\theta} = \sigma_{zz} = \sigma_{\rho z} = \sigma_{\rho\theta} = 0 \end{cases}$$

Strain energy contained in a cylinder of radius R: $E = \dfrac{\mu b^2}{4\pi}\log\left(\dfrac{R}{r_c}\right)$

Edge dislocation

$\vec{u}(\rho) \propto \log(\rho)$ $\quad \boldsymbol{\sigma} \propto \dfrac{1}{\rho}$ $\quad E = \dfrac{\mu b^2}{4\pi(1-\nu)}\log\left(\dfrac{R}{r_c}\right)$ ➔ higher energy

Infinite straight dislocation: anisotropic elasticity[1-3]

same radial variation as in isotropic elasticity but angular dependence changes (non null term)

$$\vec{u}(\rho) \propto \log(\rho) \qquad \boldsymbol{\sigma} \propto \frac{1}{\rho}$$

Strain energy contained in a cylinder of radius R: $E = \frac{1}{2} b_i K_{ij} b_j \log\left(\frac{R}{r_c}\right)$

defined by Stroh matrix K_{ij}

isotropic elasticity:

$$K_{ij} = \frac{\mu}{2\pi(1-\nu)} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1-\nu \end{pmatrix}_{(x,y,z)}$$

for z along the dislocation line (screw orientation)

1. J. D. Eshelby, W. T. Read and W. Shockley, Acta Metall. **1**, 251 (1953).

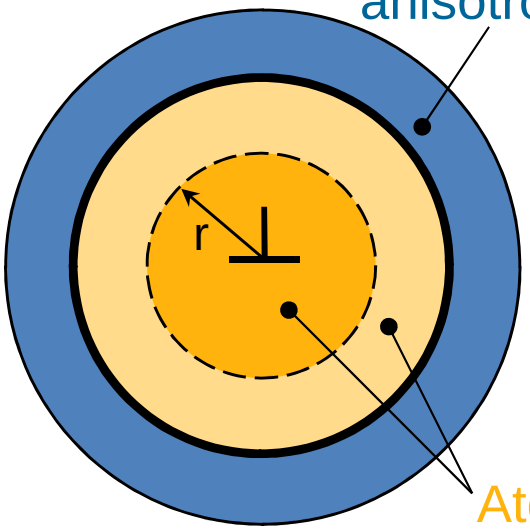
2. A. N. Stroh, Philos. Mag. **3**, 625 (1958).

3. A. N. Stroh, J. Math. Phys. (Cambridge, Mass.) **41**, 77 (1962).

2. Elasticity theory of dislocations

$\frac{1}{2}\langle 111\rangle\{110\}$ edge dislocation in Fe

Atoms fixed by linear anisotropic elasticity



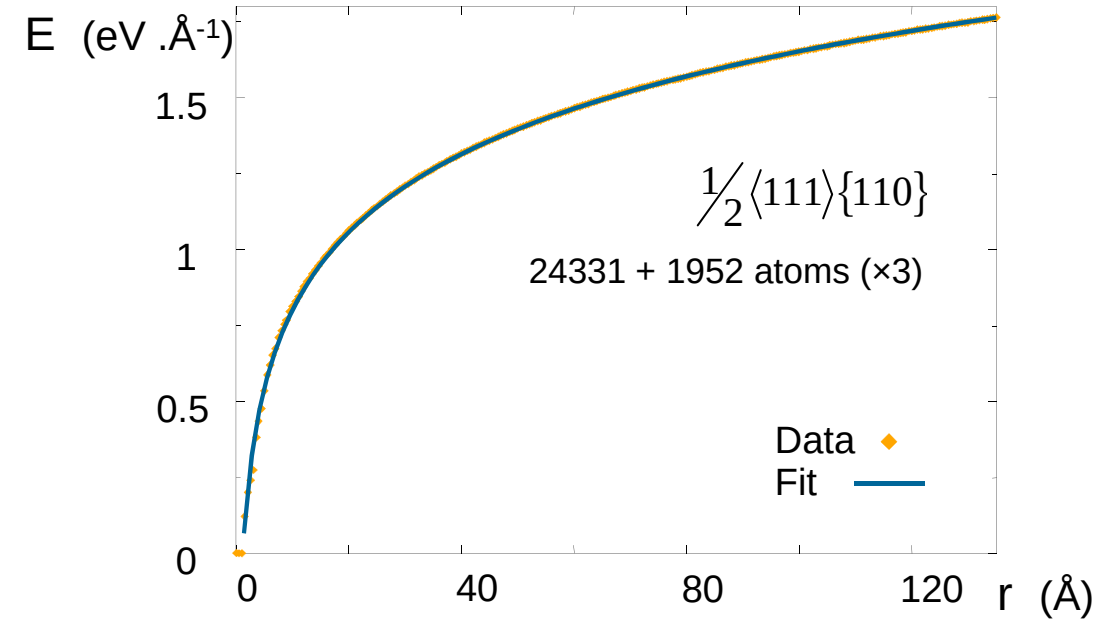
Atoms relaxed using empirical potential

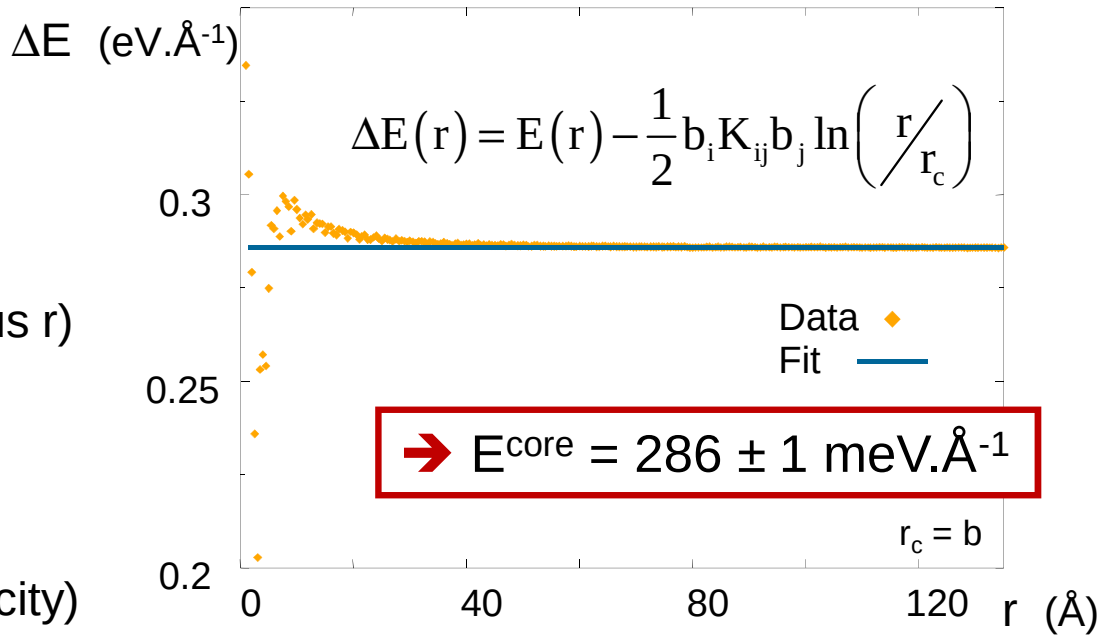
Excess energy stored in a cylinder (radius r)

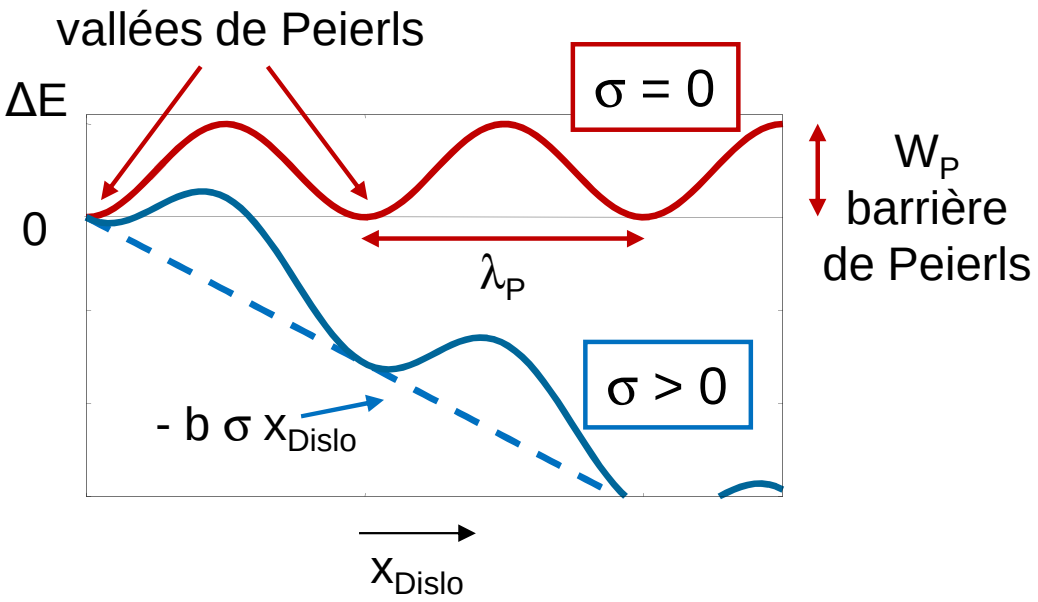
$$E(r) = E^{core} + \frac{1}{2} b_i K_{ij} b_j \ln\left(\frac{R}{r_c}\right)$$

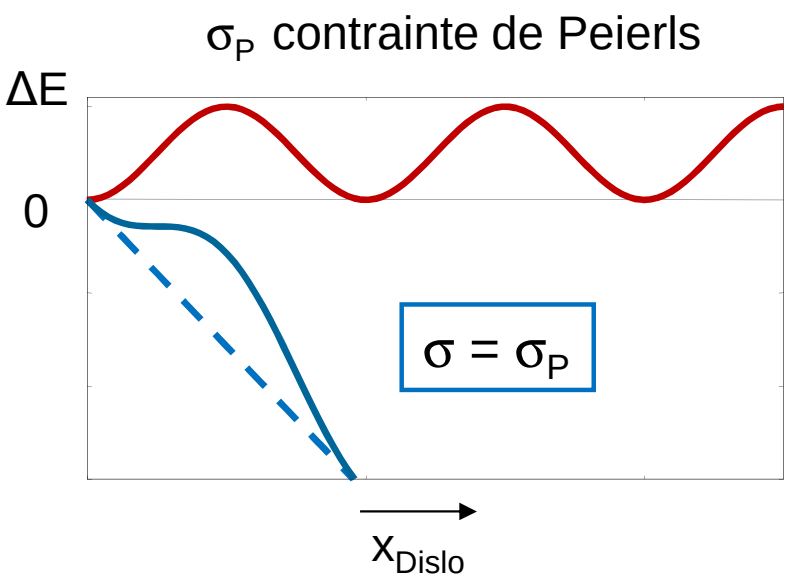
fit

known (linear anisotropic elasticity)









Dislocations:

- champ **élastique** à longue distance
- perturbation importante du réseau cristallin au voisinage de la ligne: **cœur**

Mobilité des dislocations: propriété liée au **cœur**

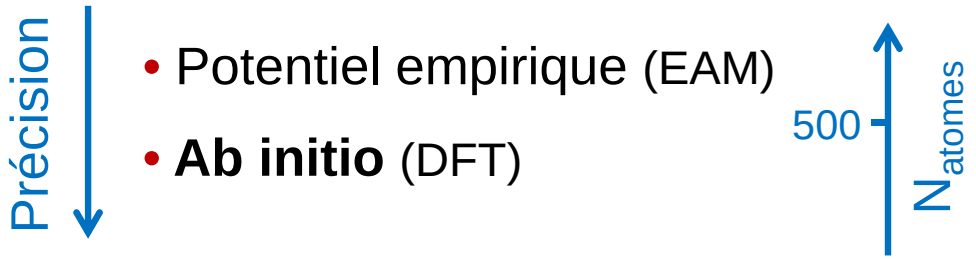
- glissement: plan de glissement, énergie et contrainte de Peierls
- montée: absorption ou élimination de défauts ponctuels
- glissement dévié: changement de plan de glissement

3. Atomistic simulations

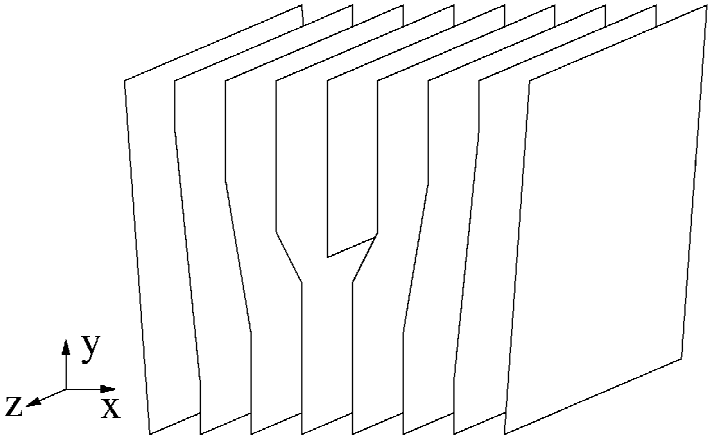
- Description de la structure du cœur des dislocations
  ➔ simulations **atomiques**
- Champ élastique à longue distance
- Séparation énergie de cœur / énergie élastique
  ➔ couplage avec théorie **élastique** (anisotrope)

Informations transposables aux échelles supérieures
(DD, plasticité cristalline…)

- plan de glissement
- énergie d'activation
- contraintes de Peierls
- lois de mobilité …



➔ need to go to a small scale to have a precise description of the atomic bonding (transition metals)

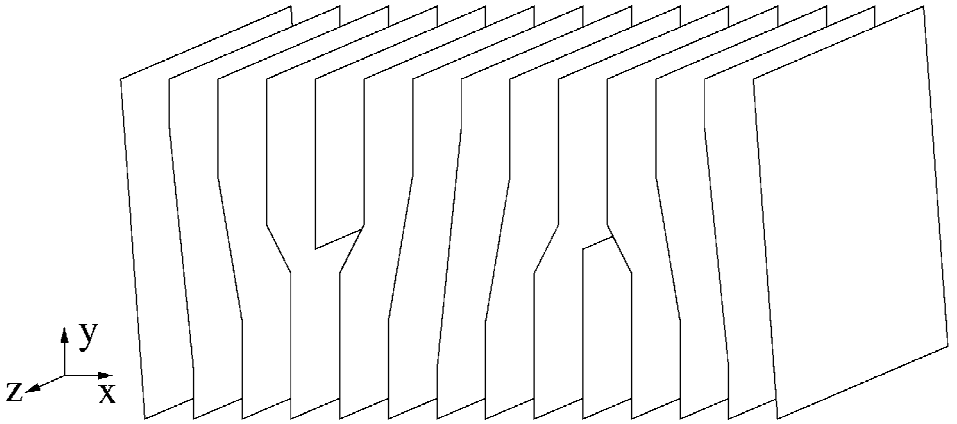


The displacement discontinuity opened by the dislocation has to be closed

➔ a simulation box with periodic boundary conditions cannot contain a single dislocation

Solutions:

- simulation box with surfaces
- dislocation dipole with PBC

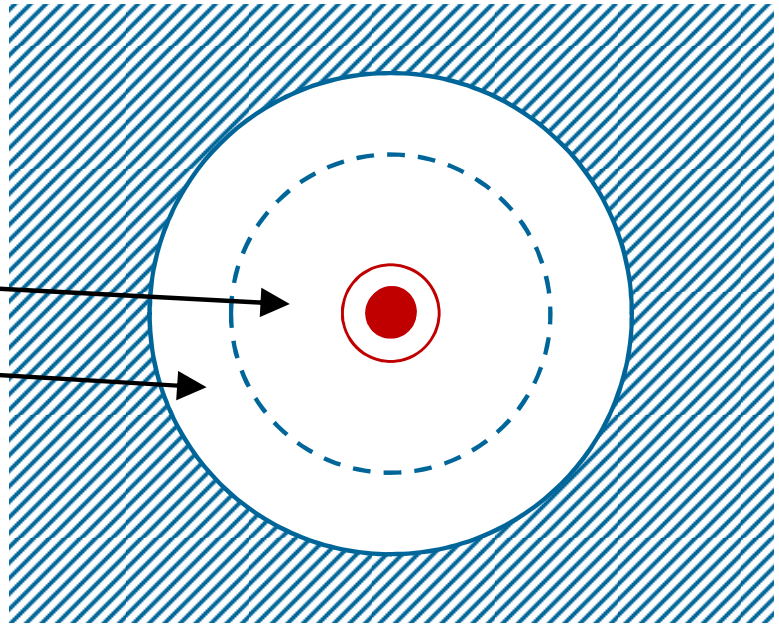


1. Cluster approach with fixed boundary

➔ **Isolated dislocation** in a cylinder

Inner atoms relaxed according to atomic forces

Outer atoms
fixed to elastic solution (Volterra)



Main drawbacks:

- the Volterra solution is only the leading term of the elastic field created by the dislocation. The core field cannot be accommodated.

$$\vec{u}(\rho) = \vec{u}_{\mathrm{V}} \log(\rho) + \mathrm{O}\left(\frac{1}{\rho}\right)$$

- back-stress exerted by the boundary when the dislocation moves.

➔ ok for empirical potentials, but not for ab initio

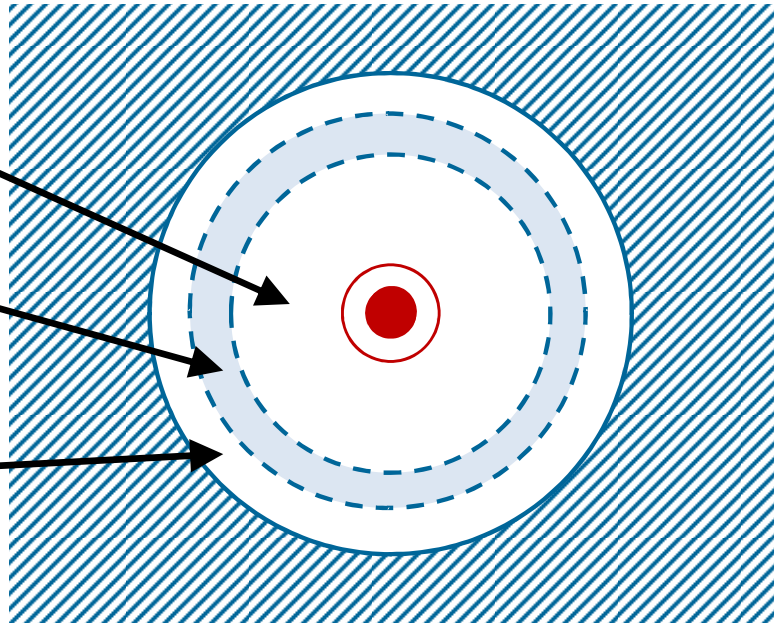
2. Cluster approach with relaxed boundary

➔ **Isolated dislocation** in a cylinder

Inner atoms relaxed according to atomic forces

Intermedidate atoms
fixed and used to calculate atomic forces due to the dislocation

Outer atoms
fixed, only here to screen the surface



Lattice Green's functions (inverse of force constants matrix) are used to relax atomic forces that build in the intermediate zone

➔ correct harmonic, thus elastic, relaxation of dislocation core

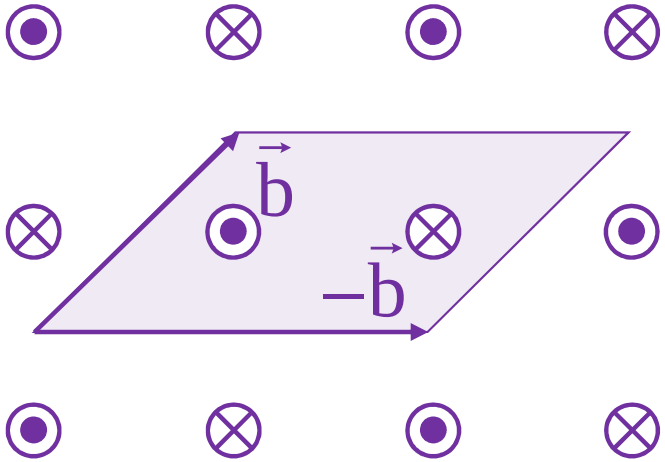
Main drawback: the energy contribution of the dislocation cannot be isolated from the surface one in ab initio calculations (no cutoff distance for atomic interactions)

➔ ok for atomic structure, for Peierls stress, but not for energy

J. E. Sinclair, P. C. Gehlen, R. G. Hoagland and J. P. Hirth, J. Appl. Phys. 49, 3890 (1978).
C. Woodward and S. I. RaoPhys. Rev. Lett. 88, 216402 (2002).
J. A. Yasi and D. R. Trinkle, Phys. Rev. E 85, 066706 (2012).

3. Dipole approach

➔ Periodic array of dislocations (periodic boundary conditions)
All atoms relaxed according to atomic forces



Main drawback: interaction between dislocations and their periodic images

➔ can be minimized with quadripolar arrangement
(but still a live)

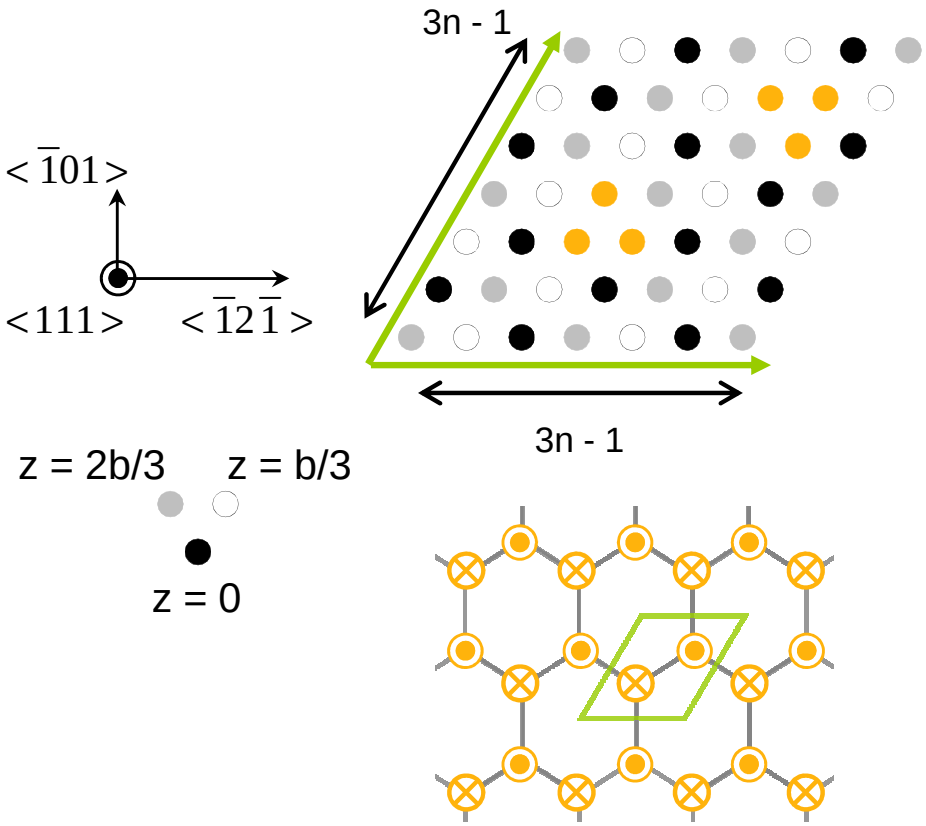
If the interaction is only caused by Volterra elastic field, it can be calculated within linear elasticity theory with proper account of PBC

Interaction energy between 2 dislocations at a distance D

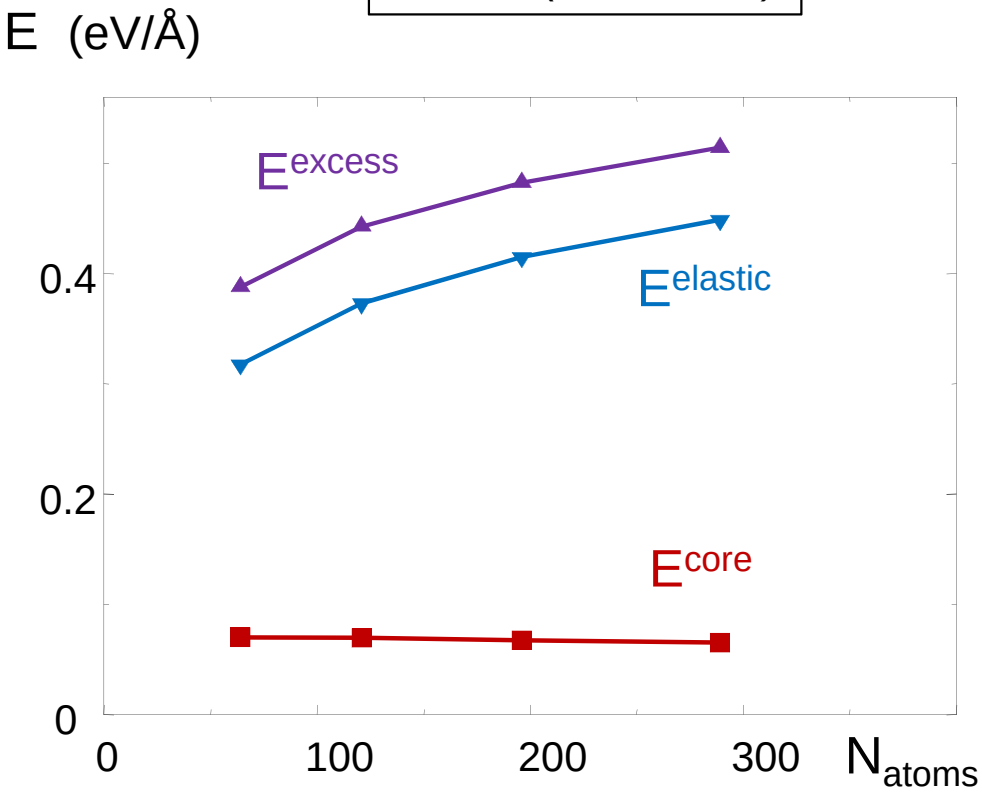
$$E^{\text{inter}} \simeq -b_i^{(1)} K_{ij} b_j^{(2)} \log\left(\frac{D}{r_c}\right)$$

W. Cai, V. V. Bulatov, J. Chang, J. Li and S. Yip, Philos. Mag. 83, 539 (2003).

3. Dipole approach



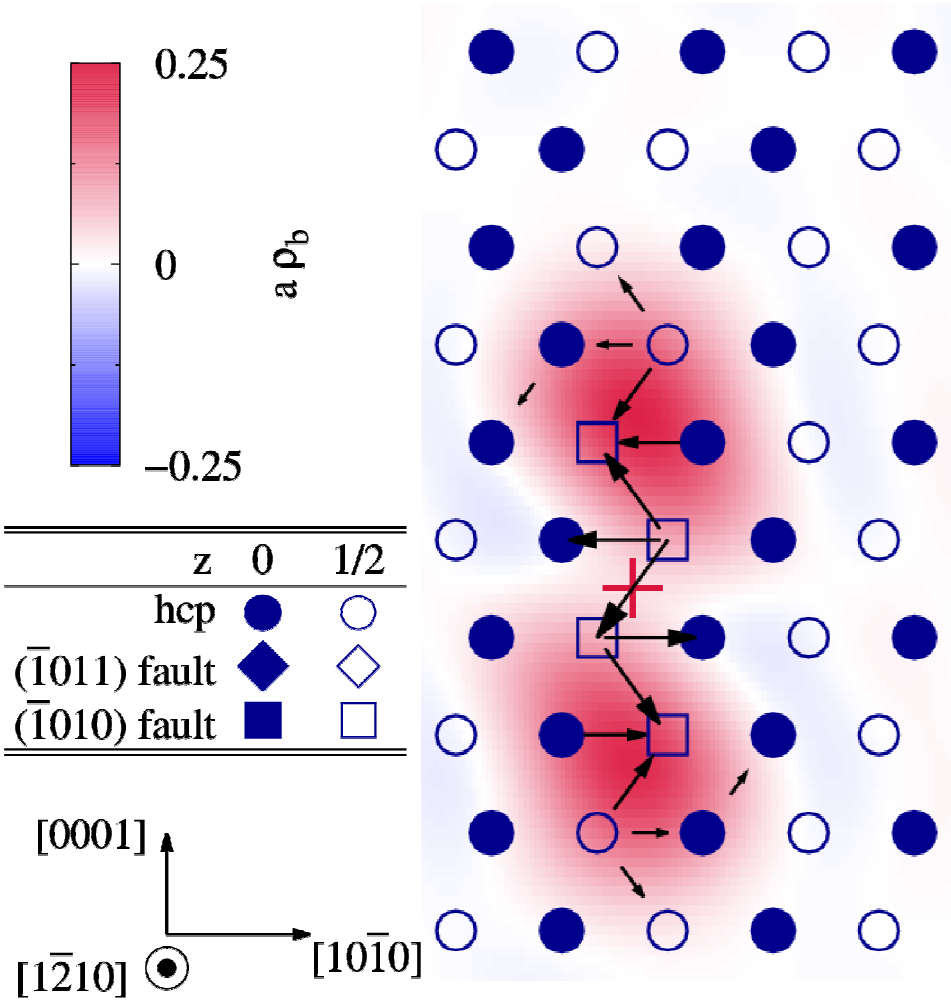
Screw dislo Fe
ab initio (L. Ventelon)



➔ core energy does not depend on simulation setup

E. Clouet, L. Ventelon and F. Willaime, Phys. Rev. Lett. 102, 055502 (2009).

Screw Dislocation in Zr: Core Structure



Differential displacement maps[1] (Vitek):

arrow proportional to difference of atomic displacement projected in the direction of the Burgers vector

➔ measure of strain

Dislocation density[2] (Nye tensor):

Nye tensor $\boldsymbol{\alpha}$ $\quad b_i = \int_A \alpha_{ij} n_j \mathrm{d}S$

α_{ij}: density of dislocation with line along direction i and Burgers vector along j

$$\boldsymbol{\alpha} = -\vec{\nabla} \times \mathbf{F}$$

with distortion $\mathbf{F}$ extracted from atomic positions

1. V. Vitek, R. C. Perrin and D. K. Bowen, Philos. Mag. **21**, 1049 (1970).

2. C. S. Hartley and Y. Mishin, Acta Mater. **53**, 1313 (2005).

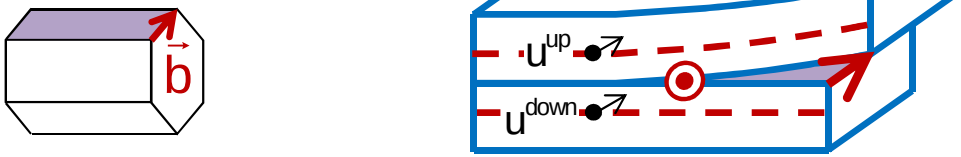
Screw Dislocation in Zr: Core Structure

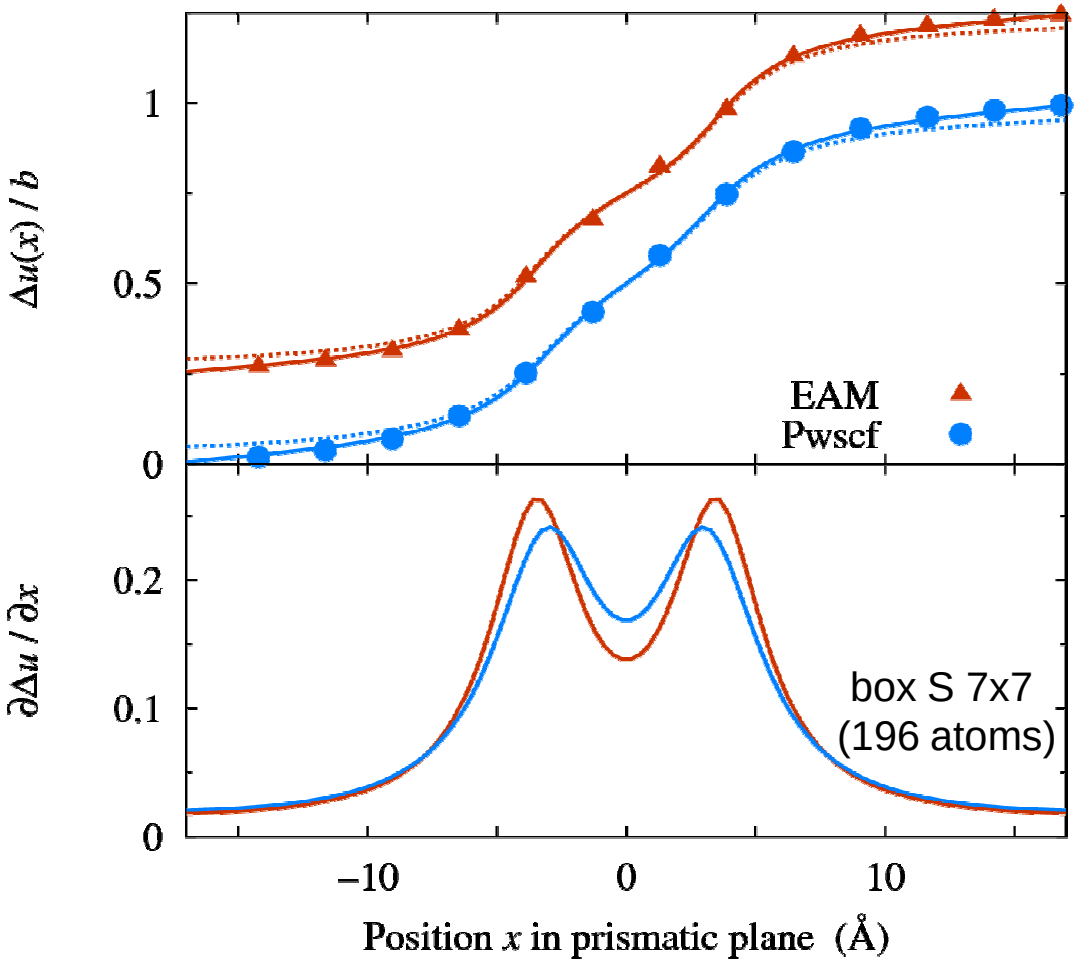
Disregistry (in prismatic plane)

1) Atomic simulations: disregristy

➔ displacement difference between above and below glide plane

$$\Delta u(x) = u^{\text{up}}(x) - u^{\text{down}}(x)$$





2) Fit **Peierls-Nabarro** model

➔ dislocation position $\mathbf{x_0}$

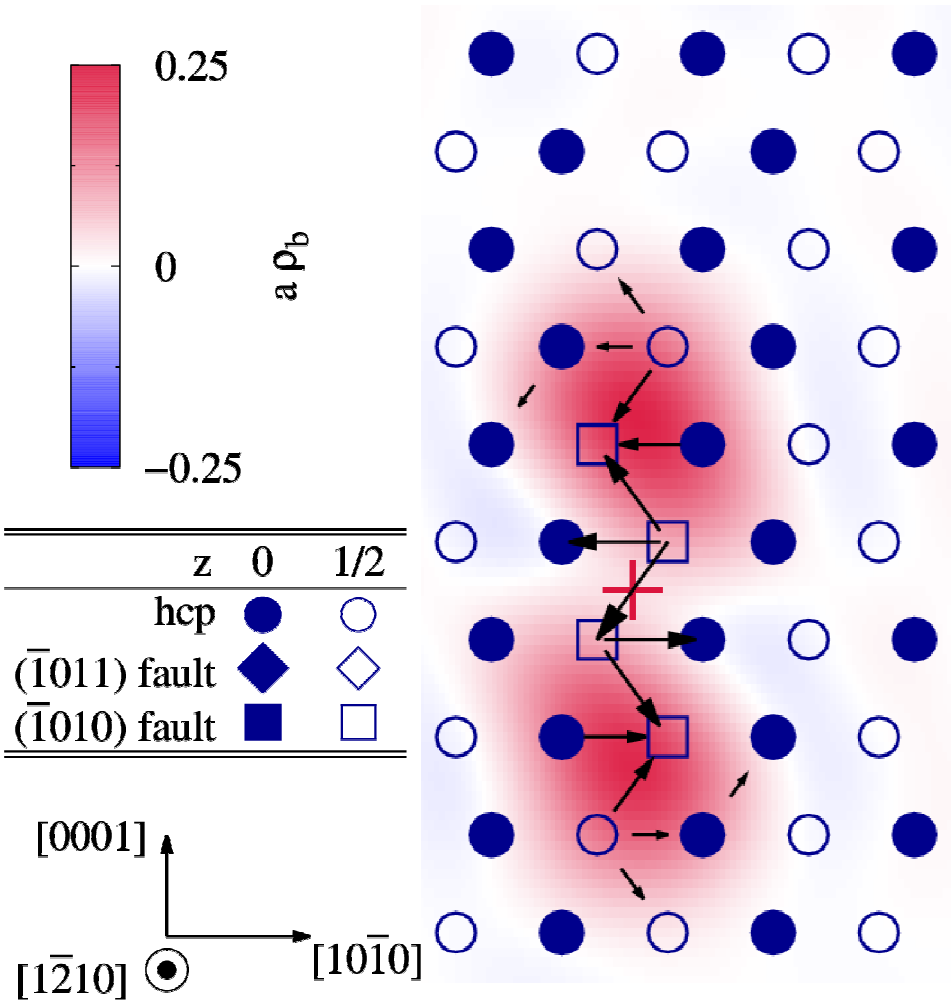
➔ dissociation length **d**

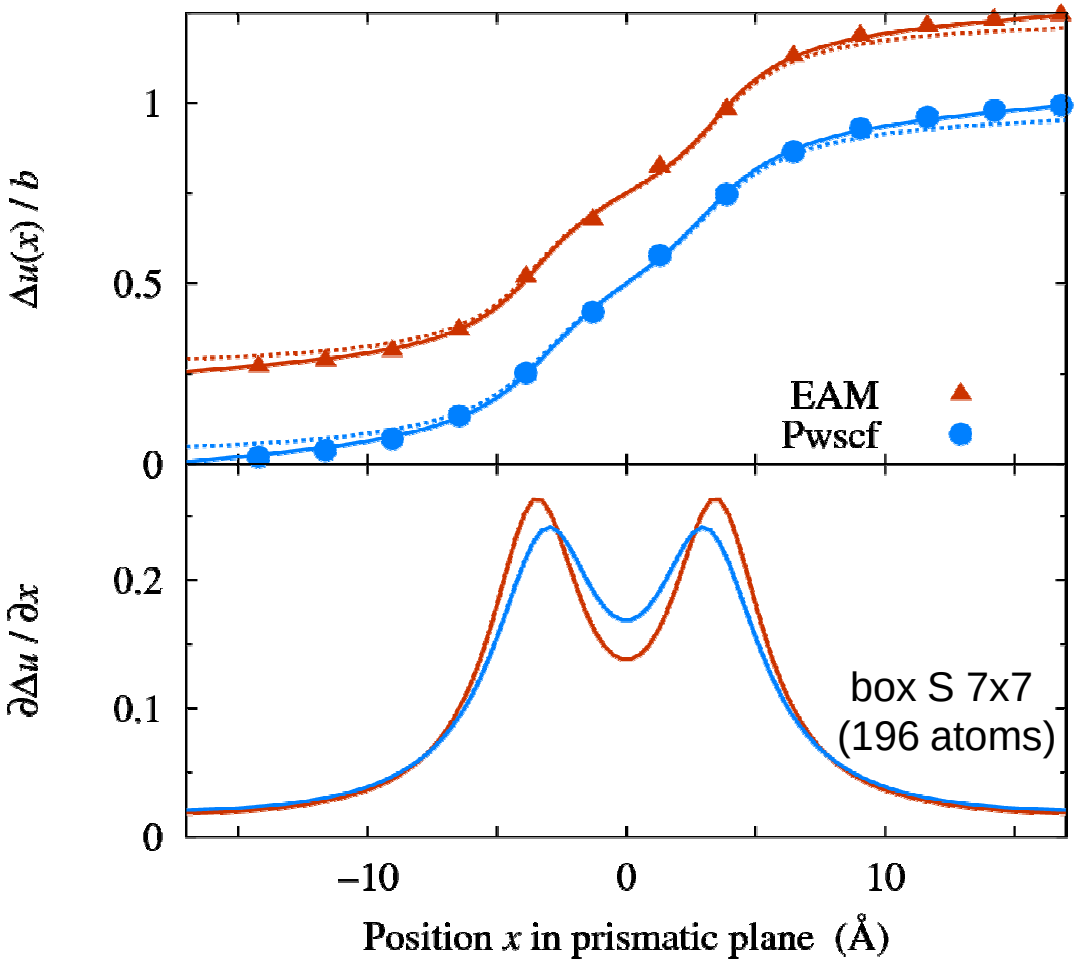
➔ partial spreading δ/π

$$\Delta u(x) = \frac{b}{2\pi}\left[\pi - \text{atan}\left(\frac{x - x_0 - d/2}{\delta}\right) - \text{atan}\left(\frac{x - x_0 + d/2}{\delta}\right)\right]$$

R. Peierls, Proc. Phys. Soc. 52, 34 (1940).
F. R. N. Nabarro, Proc. Phys. Soc. 59, 256 (1947).
D. Rodney and J. Bonneville, *Dislocations* in Pysical Metallurgy (2014).

Screw Dislocation in Zr: Core Structure





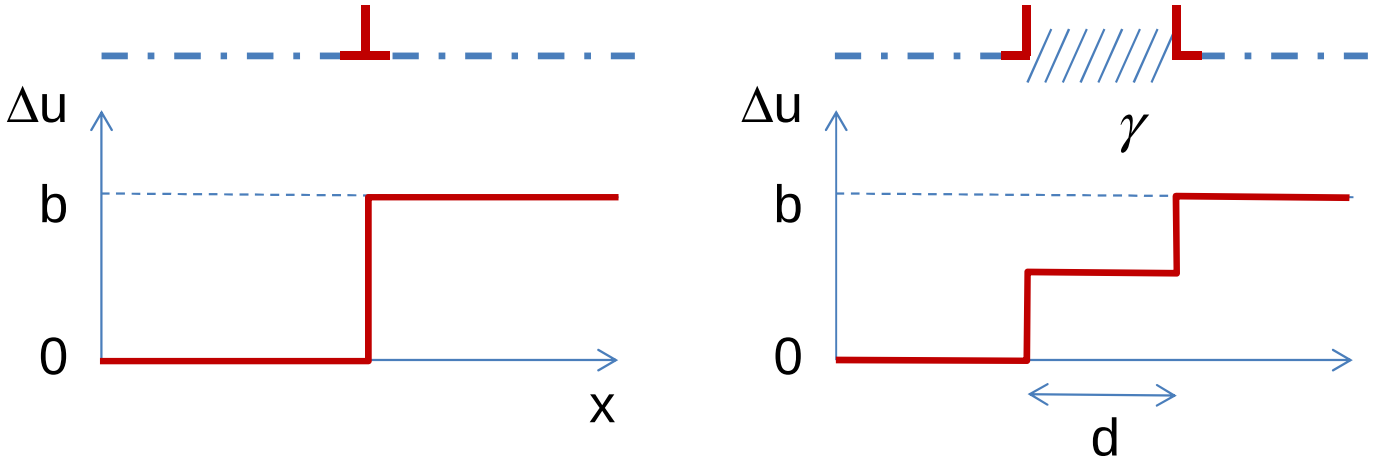
➔ **dissociation** in **prismatic** plane
in 2 partial dislocations b/2

Dislocation dissociation:

Elastic energy $E^{\mathrm{D}} \propto b^2$

$$\left\|\vec{b}^{(1)}+\vec{b}^{(2)}\right\|^2 > \left\|\vec{b}^{(1)}\right\|^2 + \left\|\vec{b}^{(2)}\right\|^2 \quad \text{if} \quad \vec{b}^{(1)}.\vec{b}^{(2)} > 0$$

➔ dissociation reduces elastic energy
… but creation of a stacking fault



Energy variation due to dissociation: $\Delta E_{\mathrm{diss}}(d) = -b_i^{(1)} K_{ij} b_j^{(2)} \ln\left(\frac{d}{r_c}\right) + \gamma d$

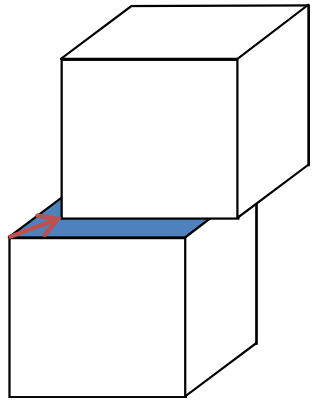
minimal for $d^{\mathrm{eq}} = \frac{b_i^{(1)} K_{ij} b_j^{(2)}}{\gamma}$

Stacking fault needs to be stable

Generalized Stacking Fault:

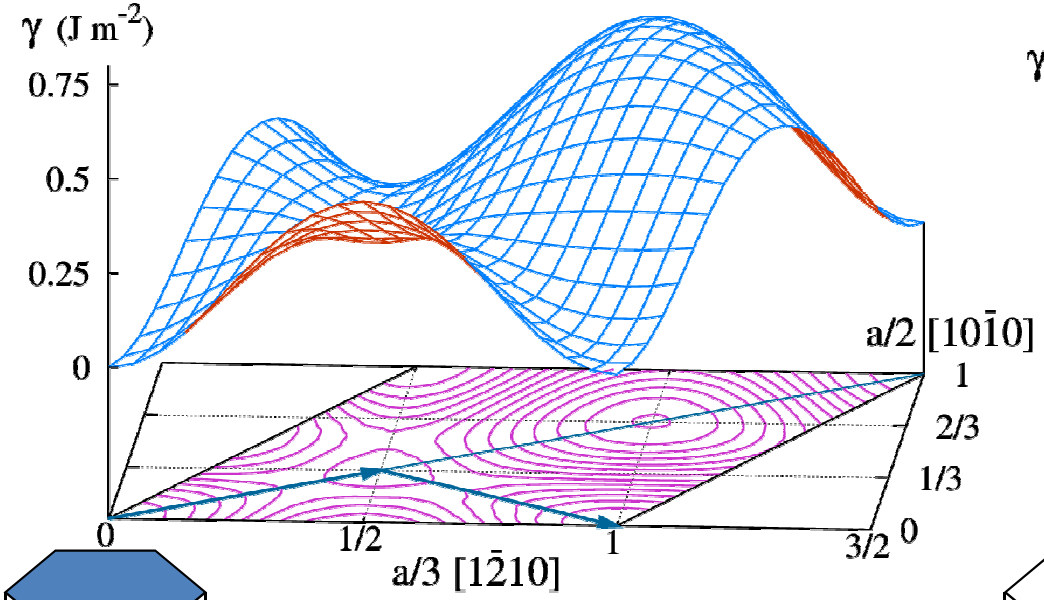
- the crystal is sheared in a plane with different fault vectors
- atoms are relaxed perpendicularly to the fault plane

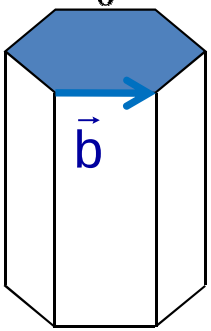
➔ look for a minimum on the surface energy



Hcp Zr

basal plane

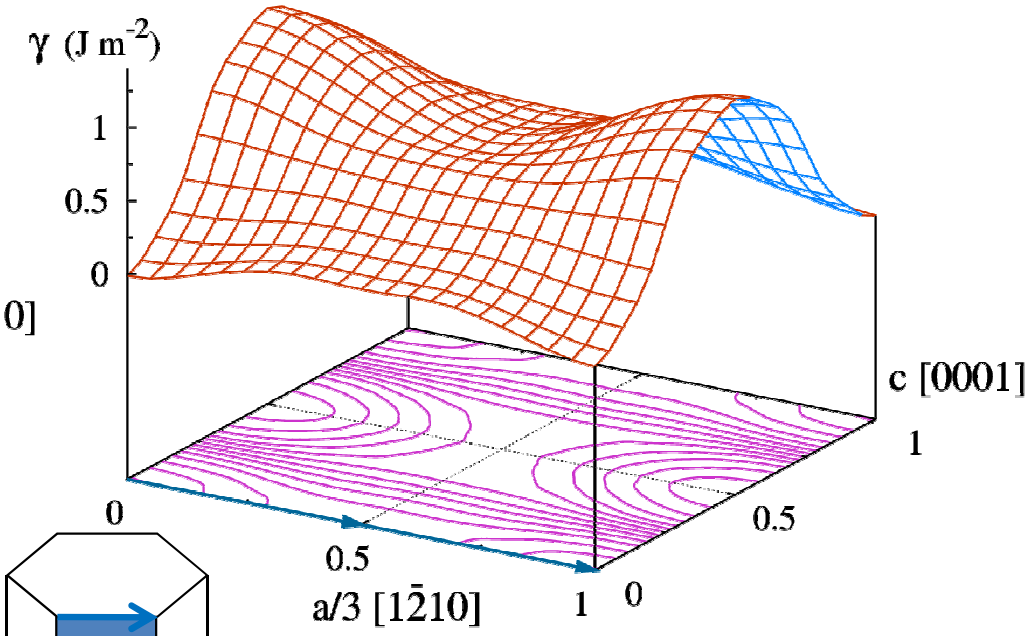


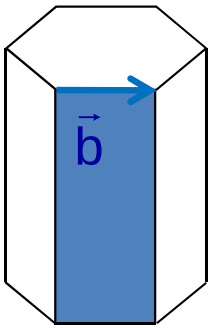


Slight minimum in 1/3[1$\bar{1}$00]

γ_b = 13.3 meV/Å^2

prism plane

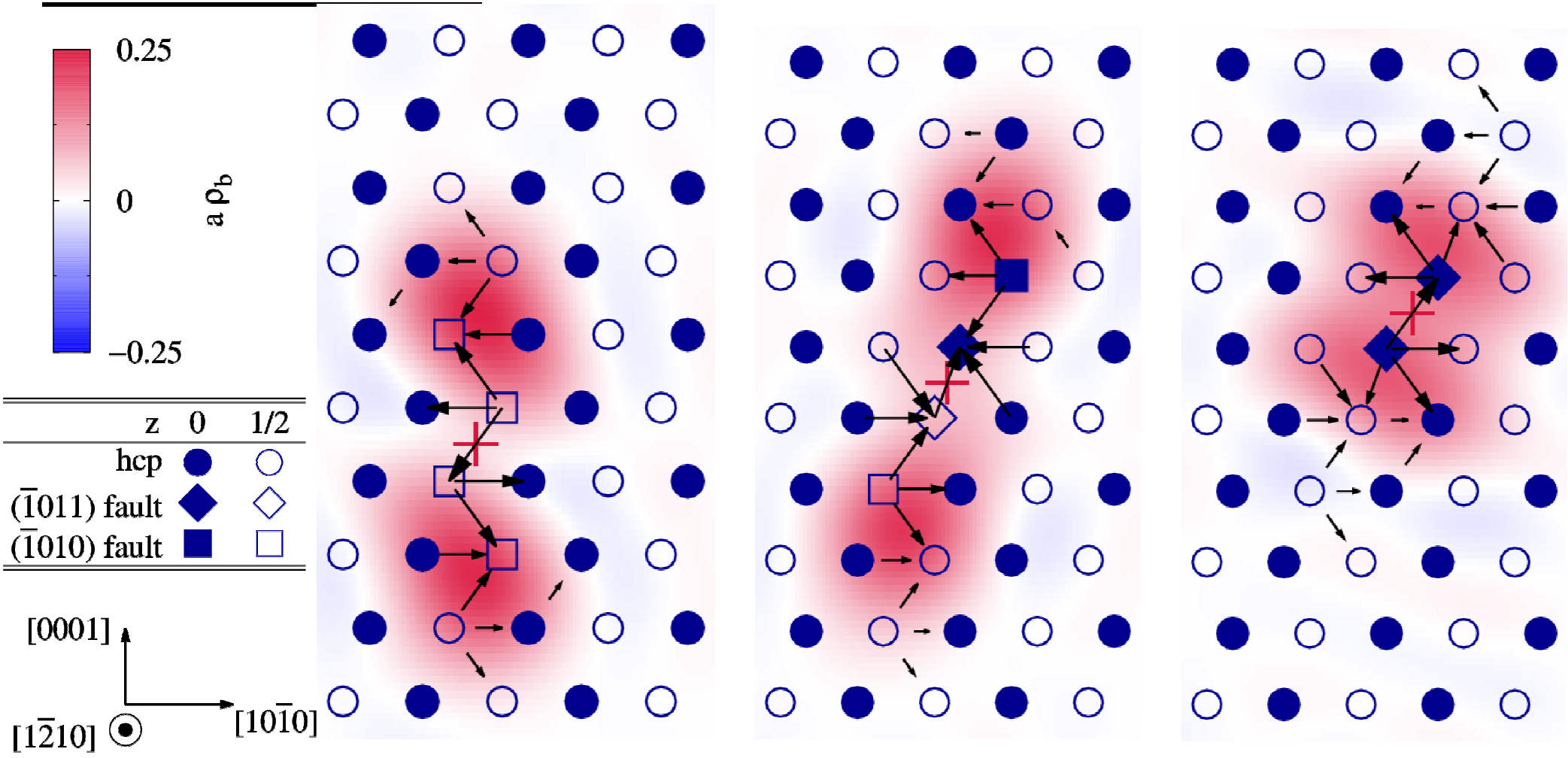




Minimun in 1/6[1$\bar{2}$10]

γ_p= 13.2 meV/Å^2

Screw Dislocation in Zr: Core Structure



Different stable core structures of the same dislocation can exist

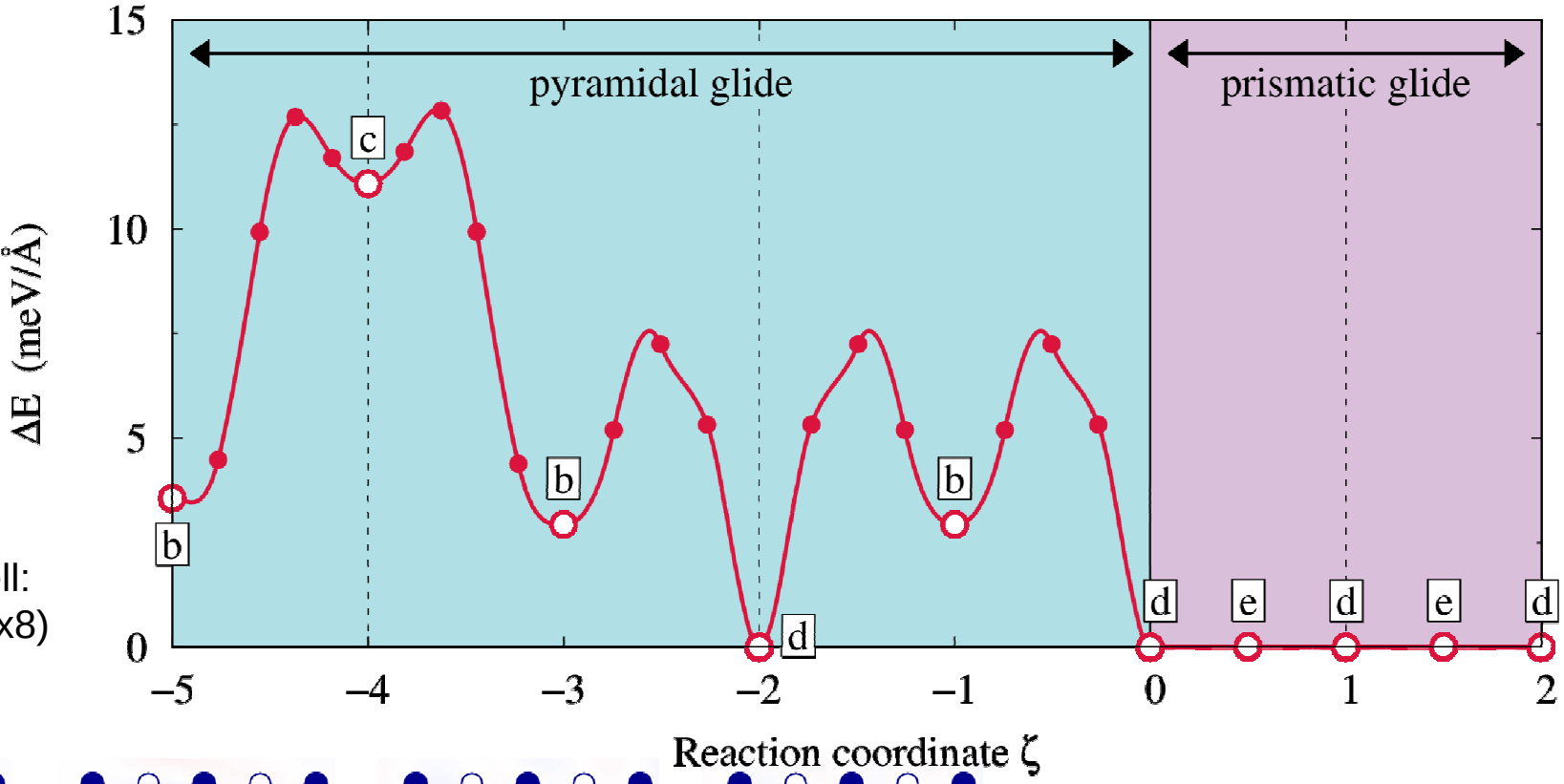
➔ need to know their energy to conclude on their stability

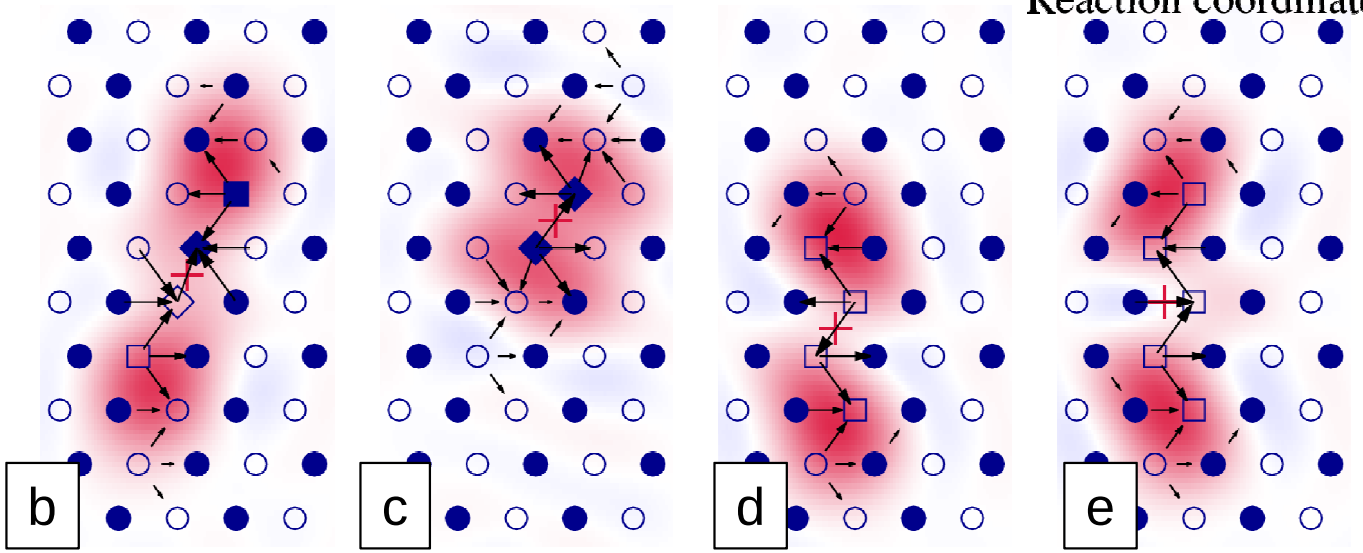
3. Atomistic simulations

Zr:

stability
mobility

Simulation cell:
192 atoms (6x8)



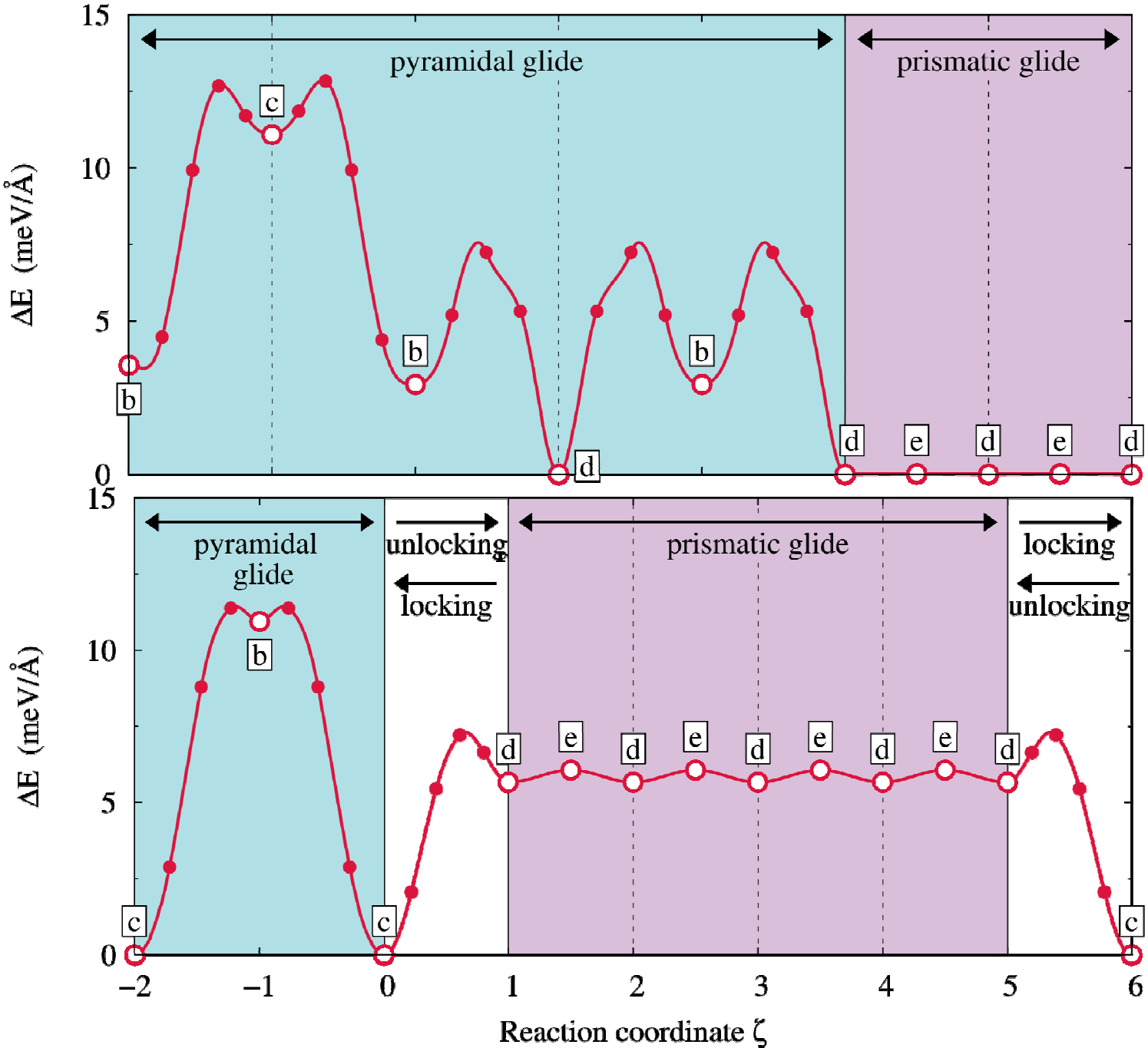


Mobility

- prismatic planes
  easy glide
- pyramidal planes (Peierls)
  nucleation of kink pairs

Zr

Ti


pyramidal glide
prismatic glide
pyramidal glide
unlocking
locking
prismatic glide
locking
unlocking
ΔE (meV/Å)
Reaction coordinate ζ
0
5
10
15
−2
−1
0
1
2
3
4
5
6
b
c
d
e

Dislocations in Zr and Ti: conclusions

screw dislocation: same configurations but different stability[5]

➔ different glide mechanisms

Zr dislocation ground state dissociated in prismatic plane

prismatic glide[1]: low Peierls stress (σ_P < 21 MPa)

easy glide in agreement with in situ TEM experiments

pyramidal and basal glide[2,3] activated above 300K

Ti dislocation ground state screw dislocation spread in pyramidal plane (fault[2,3])

prismatic glide: locking / unlocking mechanism

with a metastable glissile configuration

in agreement with locking unlocking mechanism[4] (in situ TEM experiments)

pyramidal glide: Peierls barrier (nucleation of pair of kinks) activated below 300K

1. E. Clouet, Phys. Rev. B **86**, 144104 (2012)
2. N. Chaari, E. Clouet and D. Rodney, Phys. Rev. Lett. **112**, 075504 (2014)
3. N. Chaari, E. Clouet and D. Rodney, Metall. Mater. Trans. A **45**, 5898 (2014)
4. S. Farenc, D. Caillard and A. Couret, Acta Metall. Mater. **41**, 2701 (1993); Acta Metall. Mater. **43**, 3669 (1995)
5. E. Clouet, D. Caillard, N. Chaari, F. Onimus and D. Rodney, Nature Materials in press (2015).

Acknowledgment for HPC resources

Afternoon's Conclusions

I. Elasticity Theory

II. Inclusions, Inhomogeneities and Point Defects

III. Dislocations

1. Dislocation: lattice defect
2. Elasticity theory of dislocations
3. Atomistic simulations
4. Dislocation dynamics
5. Crystal plasticity

IV. Plane interfaces