Dislocation depinning in concentrated random alloys

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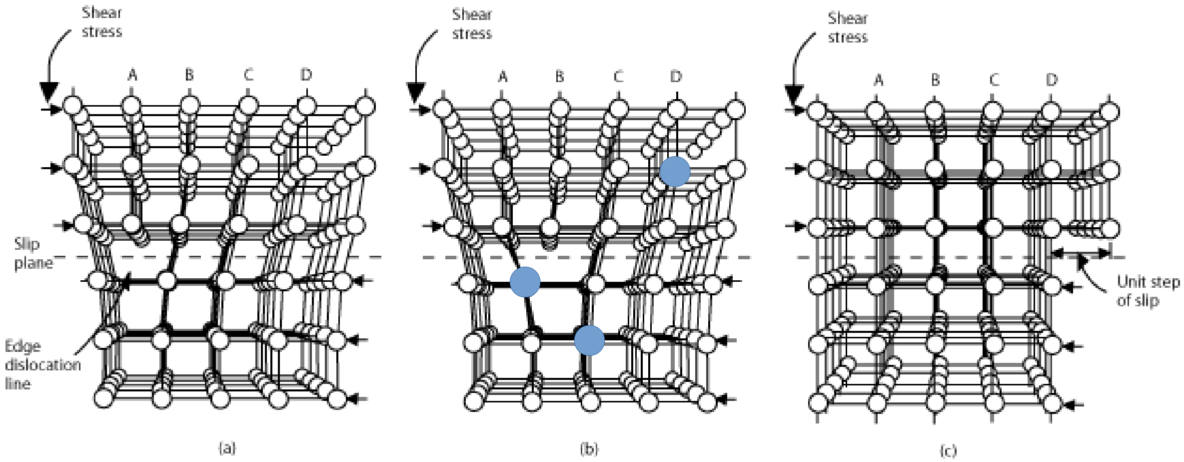
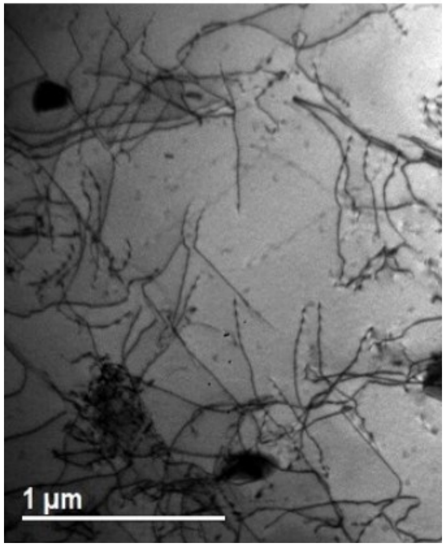
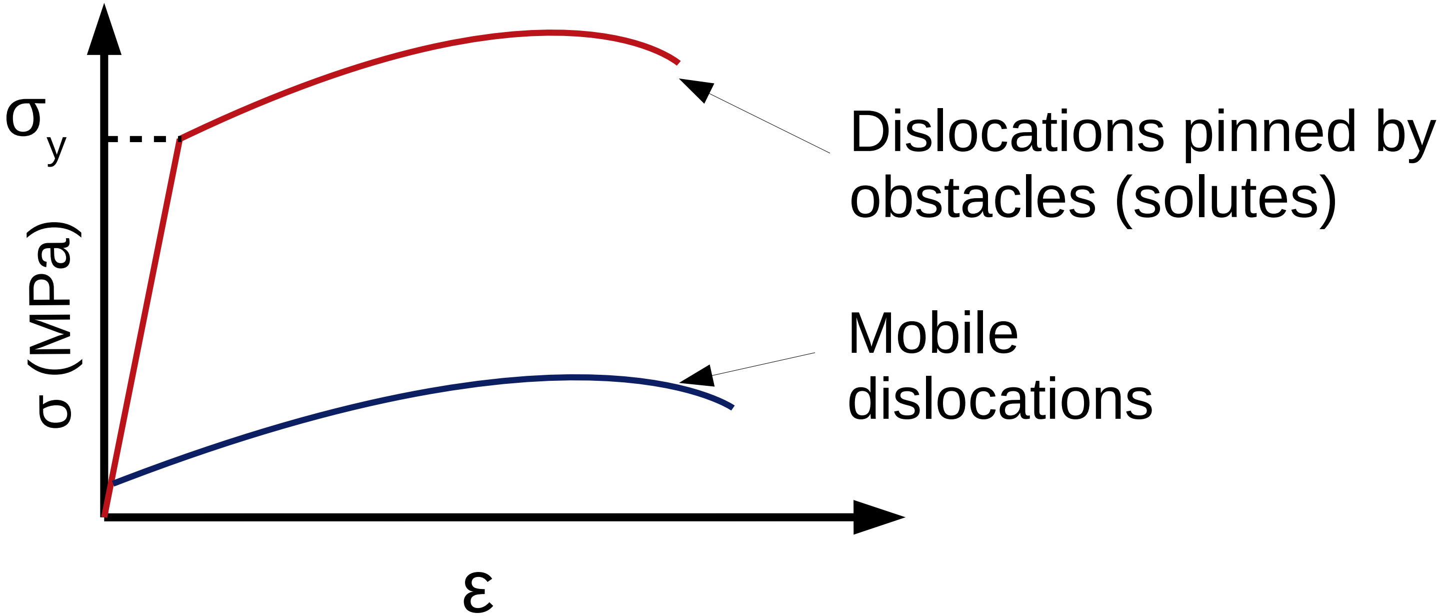
Context: dislocations and solute strengthening

- **Dislocations: linear defects in crystalline materials...**





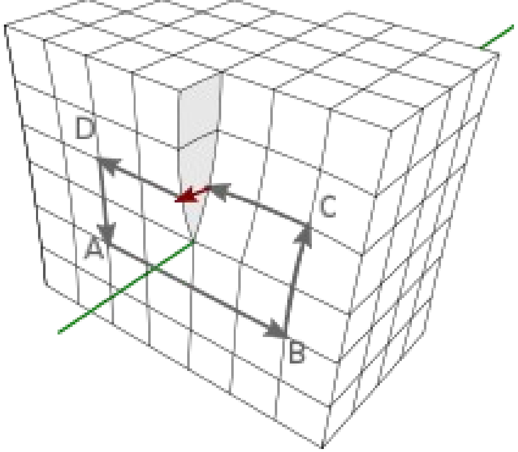
- **…that control the yield stress of the alloy**

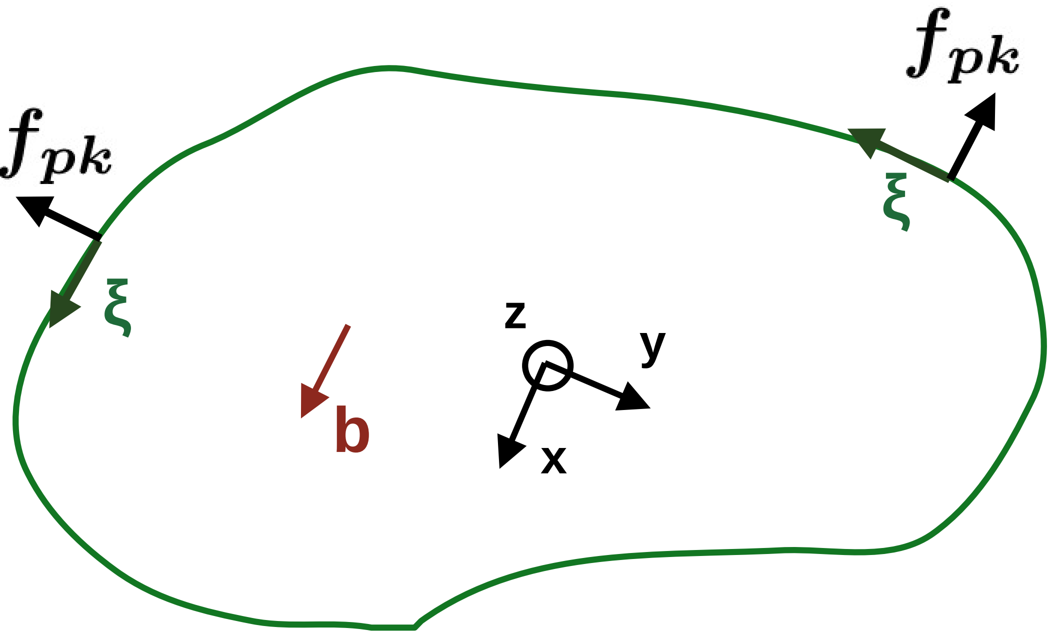


Dislocation theory

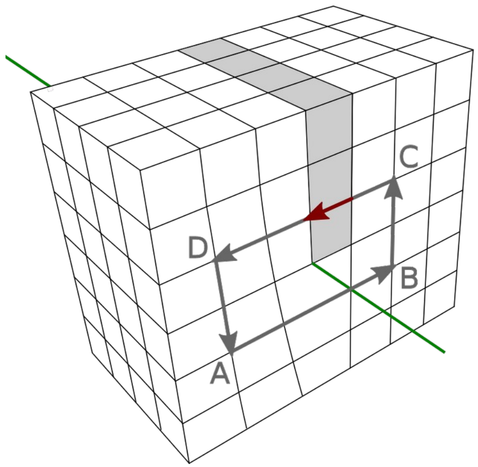
Dislocation loop

Screw dislocation





Edge dislocation

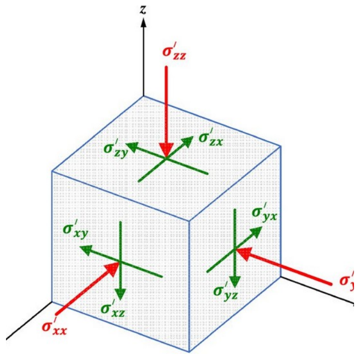


Peack-Koehler force

$$\boldsymbol{f_{pk}} = (\overline{\overline{\tau}}\boldsymbol{b}) \wedge \boldsymbol{\xi}$$

with

$$\overline{\overline{\tau}} = \begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \tau_{yy} & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \tau_{zz} \end{bmatrix}$$



$$\boldsymbol{f_{pk}} \cdot \boldsymbol{x} = -\boxed{\tau_{xz}} b_x \xi_y$$

$$\boldsymbol{f_{pk}} \cdot \boldsymbol{y} = \boxed{\tau_{xz}} b_x \xi_x$$

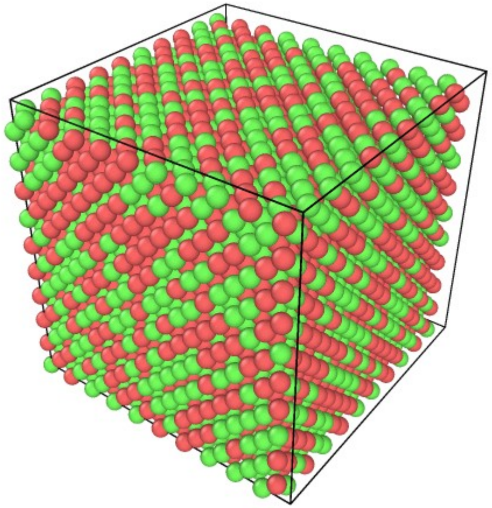
(dislocation is confined in a plane)

What do the stress field look like in random alloys ? $\tau_{xz}(x, y)$ **?**

Outline

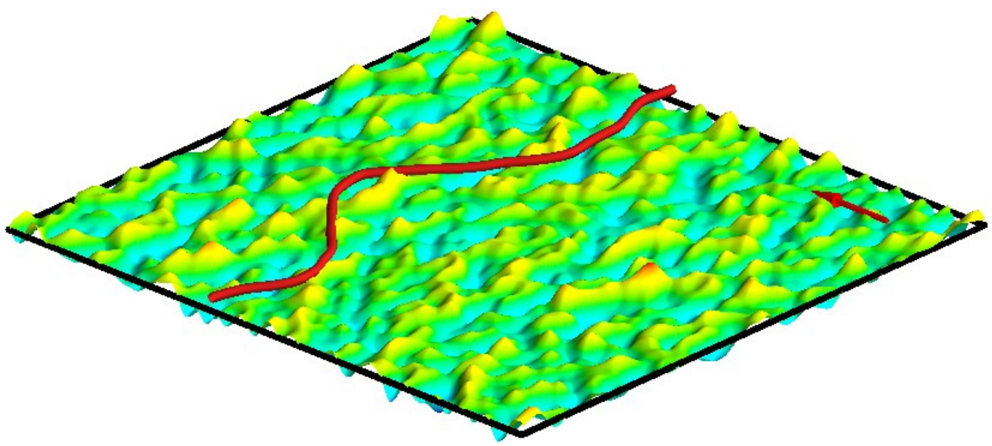
1. Characterize the stress field in random alloys

- Variance
- Correlations



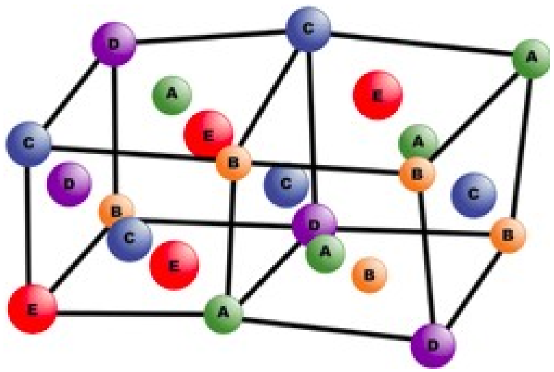
2. Analyze dislocation depinning in this random stress

- Edge
- Screw
- Mixed 45^{o}

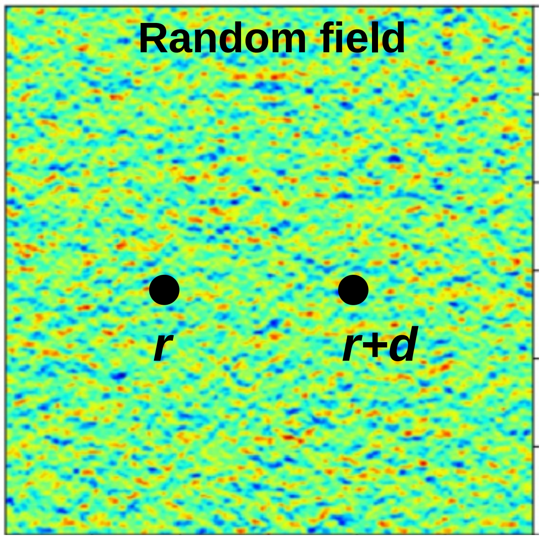


Elastic fields in random alloys

Concentrated random alloy



- **Displacement field** $u_i(\boldsymbol{r})$
- **Strain field** $\varepsilon_{ij}(\boldsymbol{r})$
- **Internal stress field** $\tau_{ij}(\boldsymbol{r})$



Variances:

$\langle u^2 \rangle$ $\langle \varepsilon^2 \rangle$ **- can be measured experimentally (XRD,TEM) [1]**

$\langle \tau^2 \rangle$ **- responsible for pinning dislocations**
- not easily measurable

Correlations:

$$\langle u_i(\boldsymbol{r}) u_i(\boldsymbol{r}+\boldsymbol{d}) \rangle$$

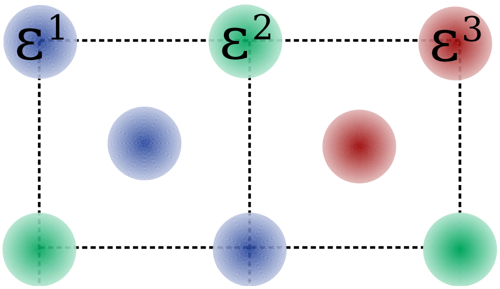
$$\langle \varepsilon_{ij}(\boldsymbol{r}) \varepsilon_{ij}(\boldsymbol{r}+\boldsymbol{d}) \rangle$$

$$\langle \tau_{ij}(\boldsymbol{r}) \tau_{ij}(\boldsymbol{r}+\boldsymbol{d}) \rangle$$

[1] Zhang, Yong, et al. Progress in Materials Science 61 (2014): 1-93.

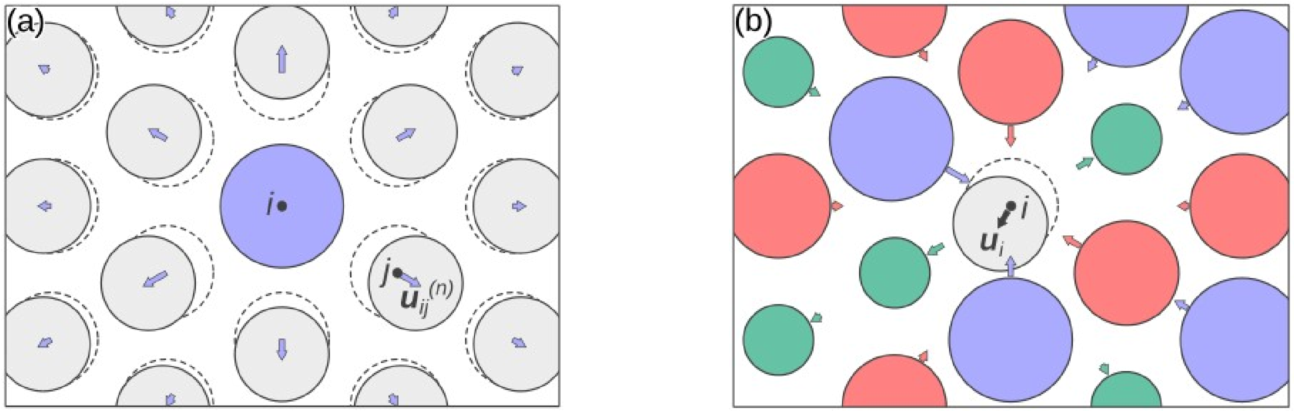
Elastic model of random alloys

- **1 atom = 1 Eshelby inclusion in an isotropic continuous medium**



$$\overline{\overline{\varepsilon}}^{\alpha} = \varepsilon^{\alpha} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

[Noehring, Curtin, Scripta Mat. 168, 2019]



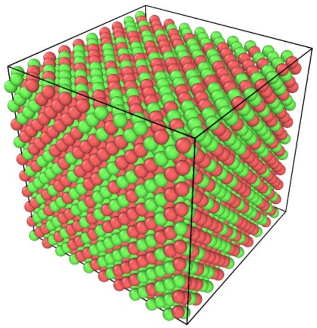
Displacements:

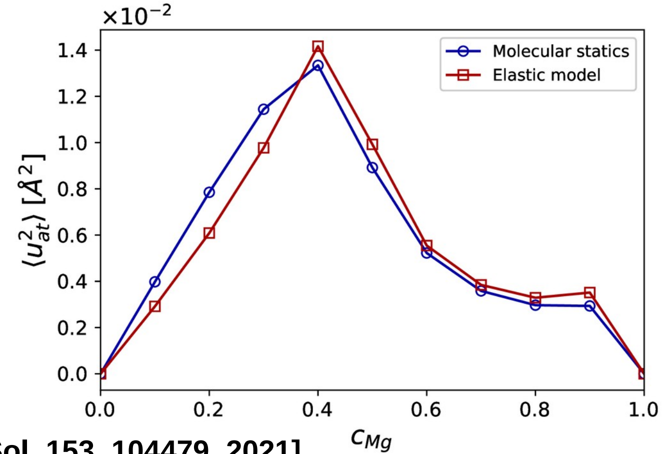
$$\boldsymbol{u}^{Eshelby}(\boldsymbol{r}) = \varepsilon \frac{v_{at}}{4\pi} \frac{1+\nu}{1-\nu} \frac{\boldsymbol{r}}{|\boldsymbol{r}|^3} \qquad \langle u^2 \rangle = \frac{25.3}{16\pi^2} \frac{v_{at} \sum_\alpha c_\alpha \varepsilon_\alpha^2}{a_{lat}} \left(\frac{1+\nu}{1-\nu} \right)^2$$

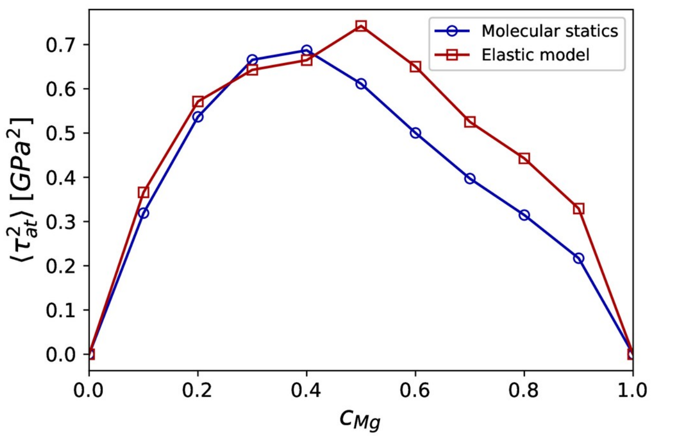
Shear stresses:

$$\tau_{ij}^{Eshelby}(\boldsymbol{r}) = -\varepsilon \frac{3 v_{at} \mu}{2\pi} \frac{1+\nu}{1-\nu} \frac{r_i r_j}{\boldsymbol{r}^5} \qquad \langle \tau^2 \rangle = \frac{81.16}{16\pi^2} \frac{v_{at} \mu^2 \sum_\alpha c_\alpha \varepsilon_\alpha^2}{a_{lat}^3} \left(\frac{1+\nu}{1-\nu} \right)^2$$

- **Al-Mg alloy**



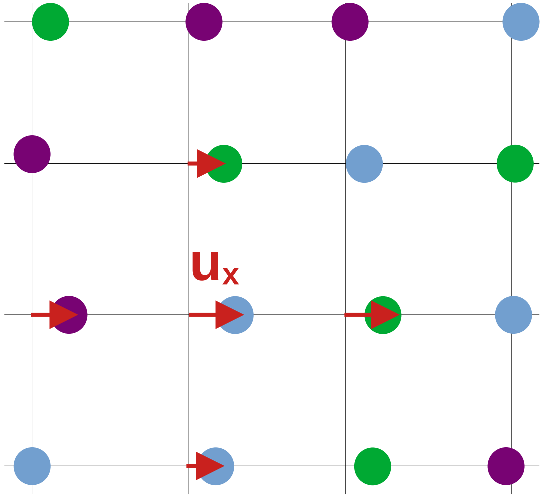




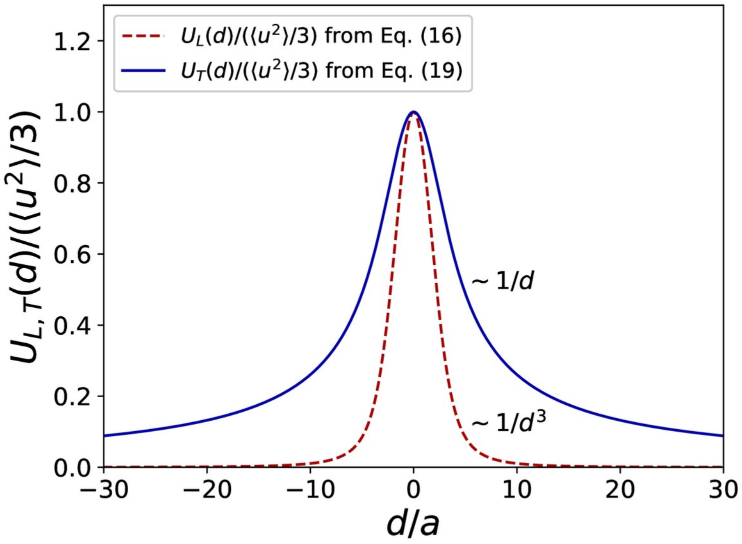
[P-A Geslin, D. Rodney, J. Mech. Phys. Sol. 153, 104479, 2021]

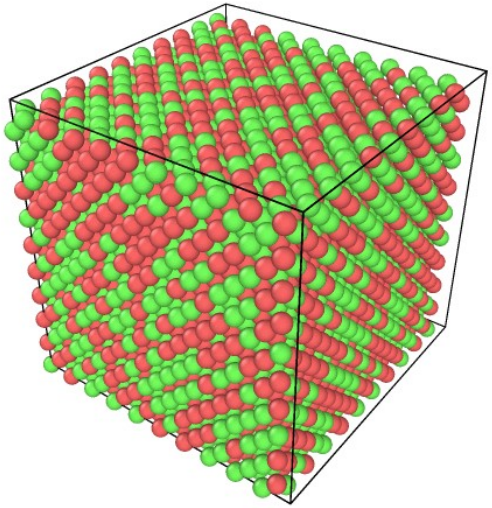
Displacement correlations

- **Displacement correlations**

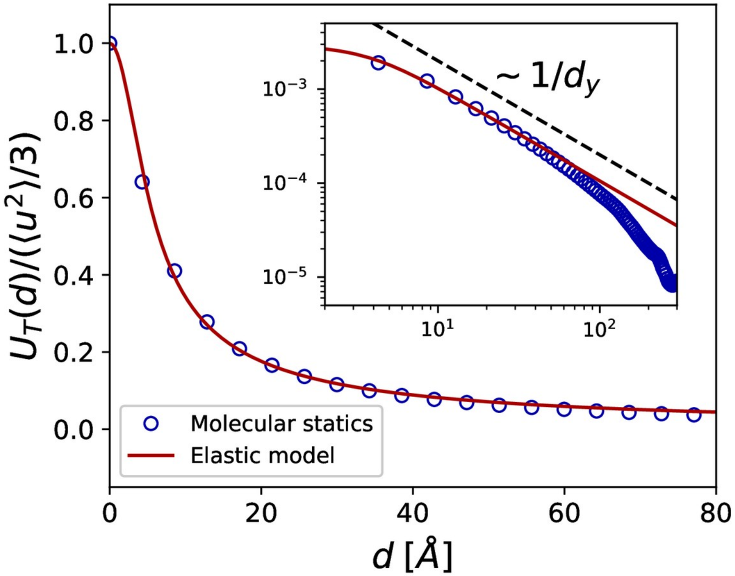


- **Elastic model prediction**



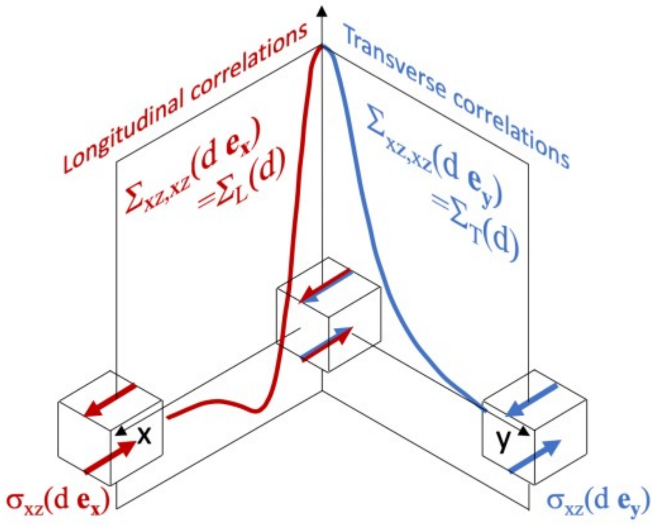


- **Atomistic Al-Mg**

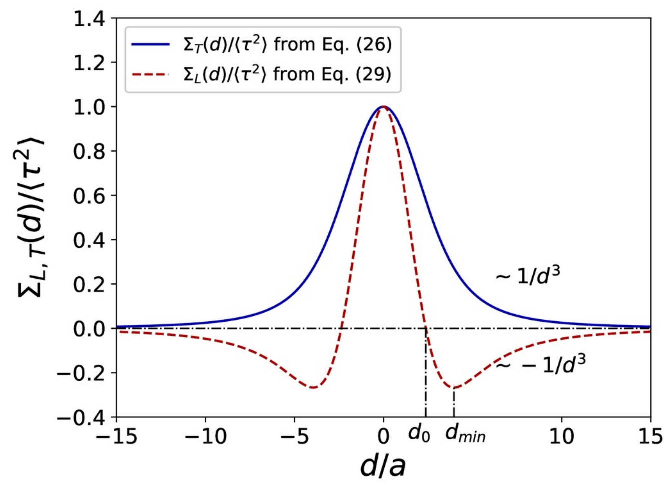


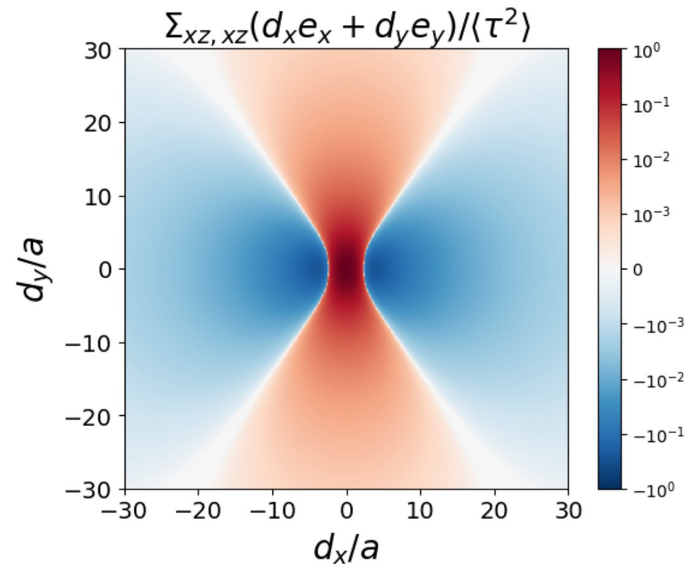
Shear stress field correlations

$$\Sigma_{xz,xz}(\boldsymbol{d}) = \langle \tau_{xz}(\boldsymbol{r})\tau_{xz}(\boldsymbol{r}+\boldsymbol{d})\rangle$$

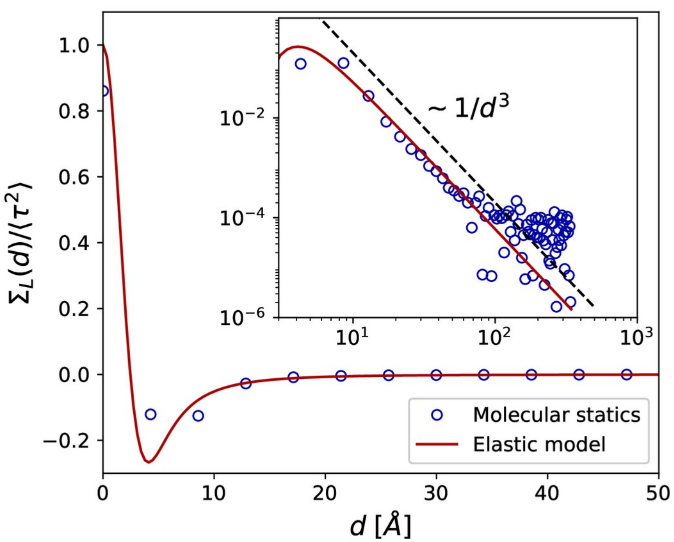


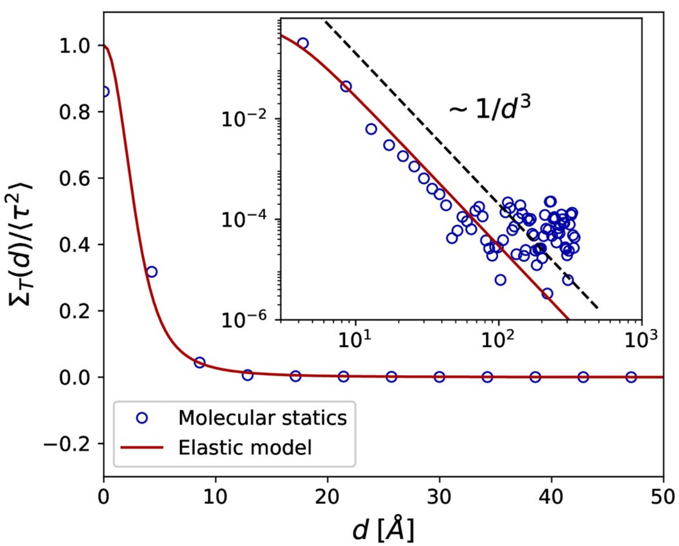
➢ **Elastic model prediction**

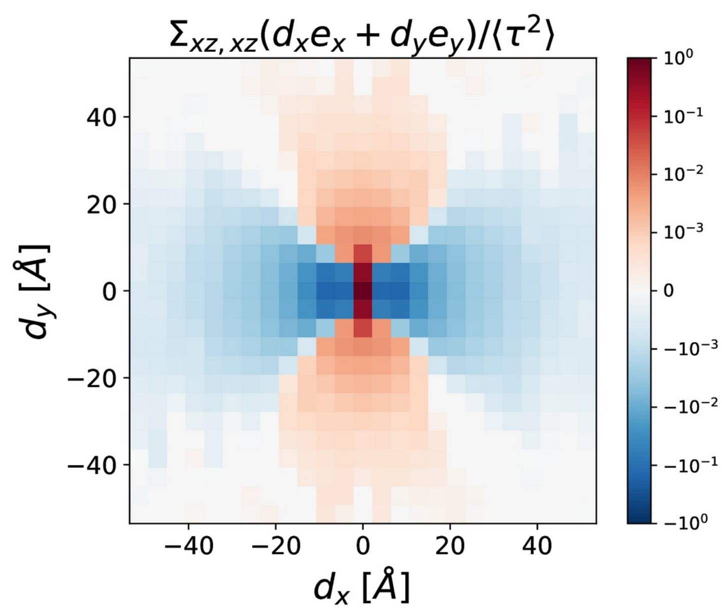




➢ **Al-Mg system**





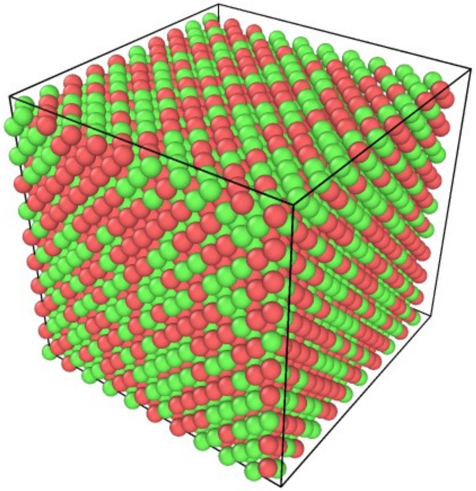


[P-A Geslin, D. Rodney, J. Mech. Phys. Sol. 153, 104480, 2021]

Outline

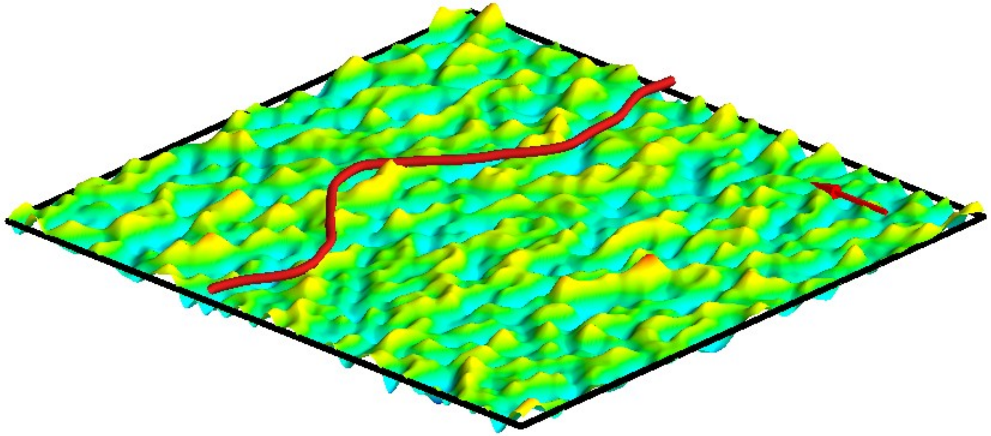
1. Characterize the stress field in random alloys

- Variance
- Correlations

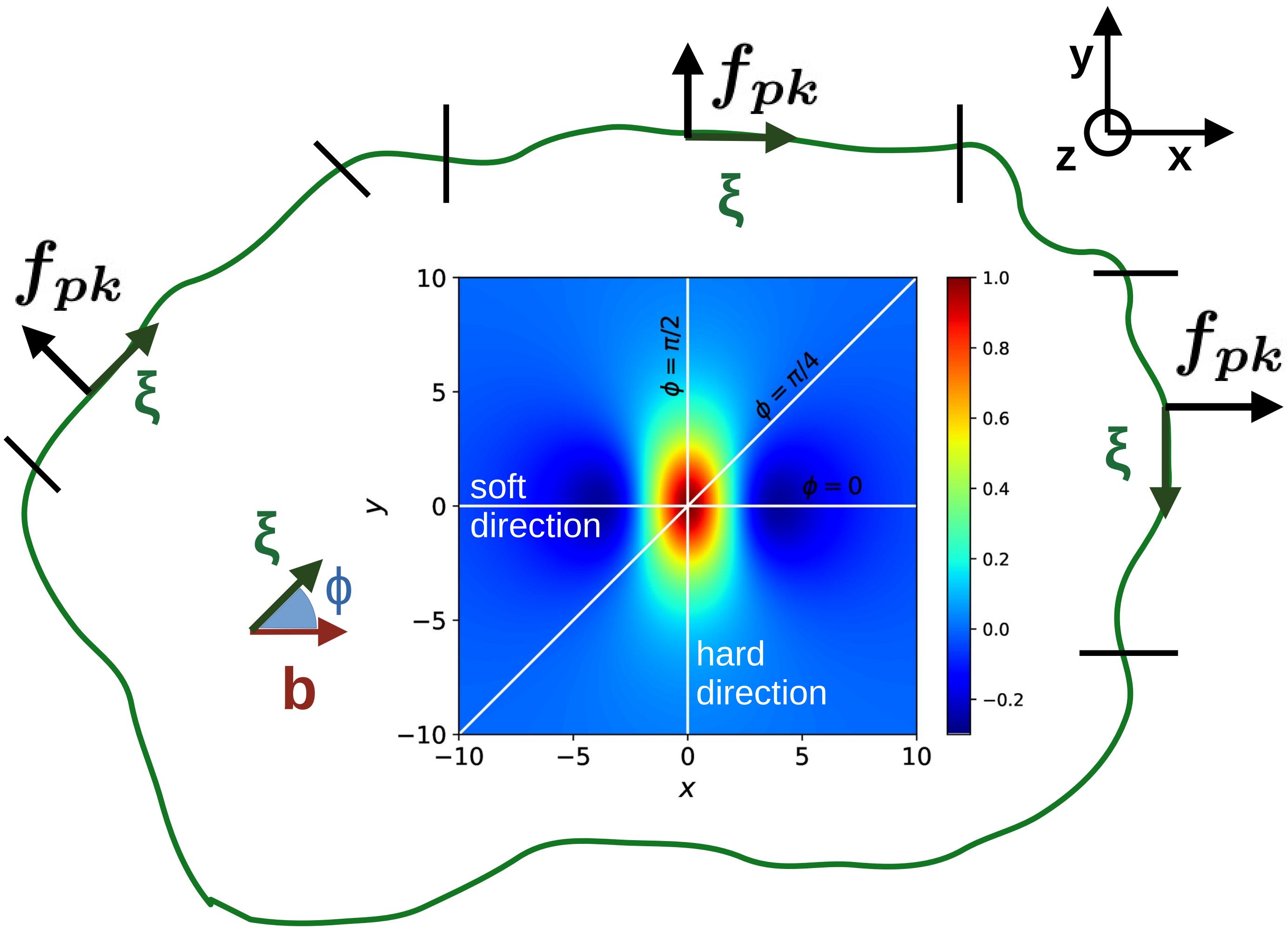


2. Dislocation depinning in this random stress

- Edge
- Screw
- Mixed 45^{o}

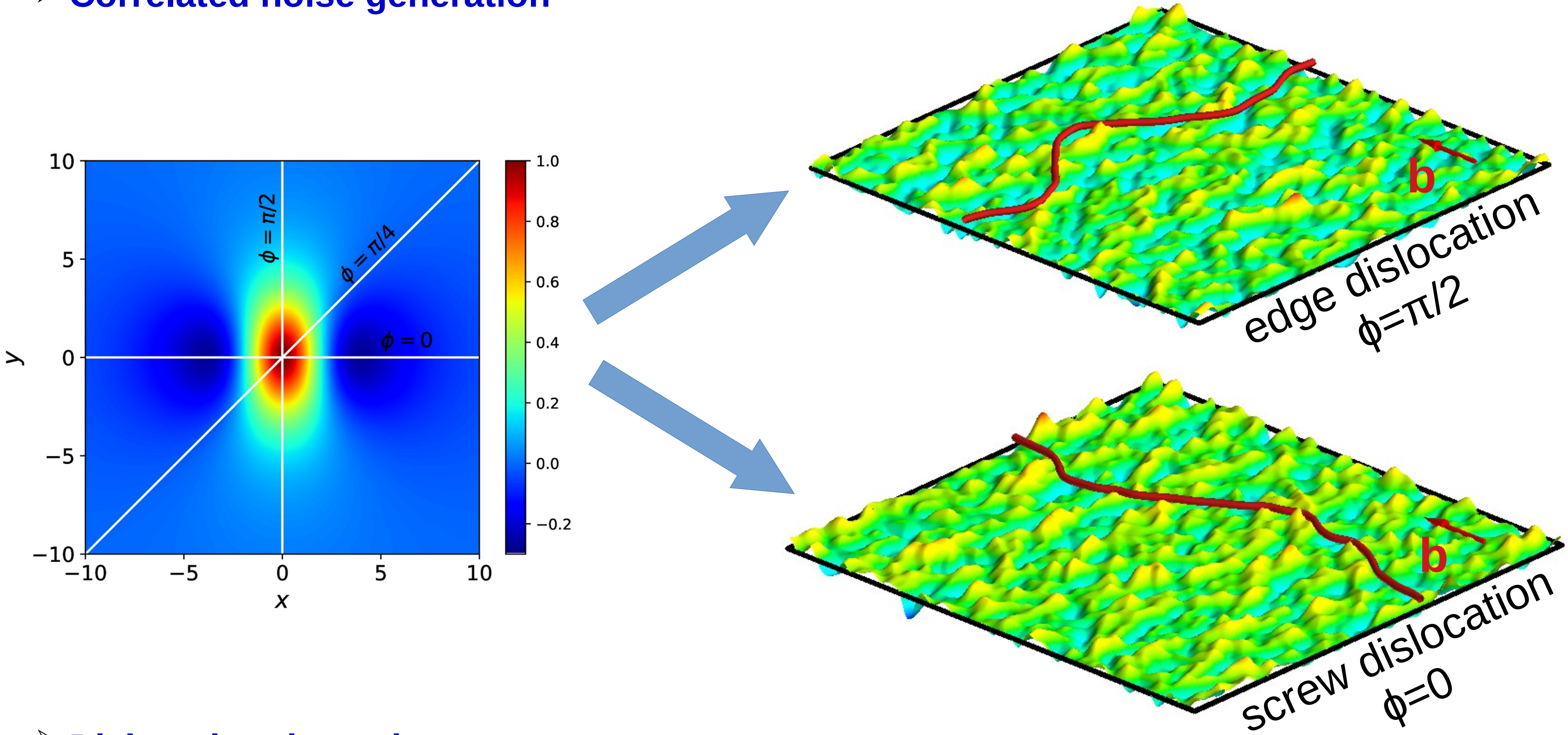


Dislocation depinning in correlated noise



Dislocation depinning in correlated noise

- **Correlated noise generation**

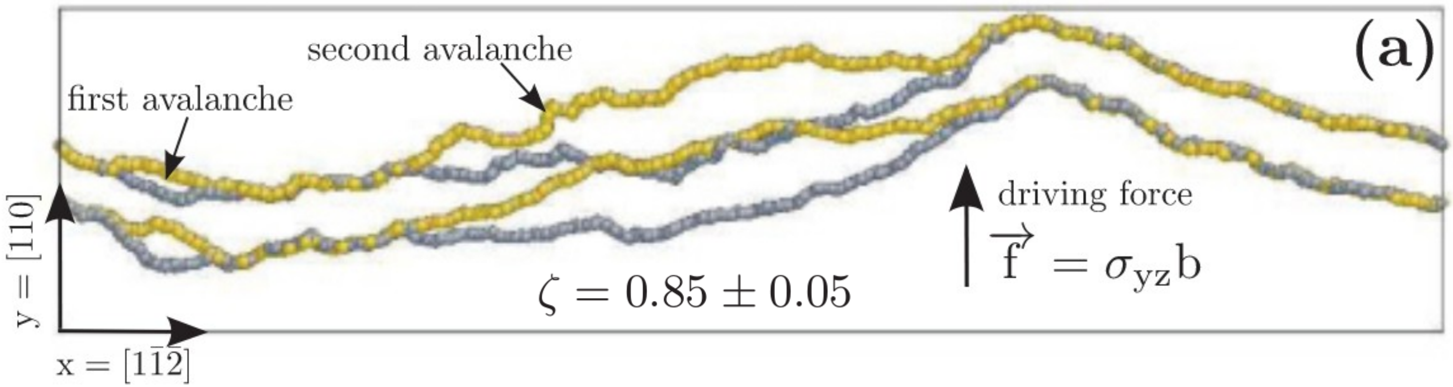


- **Dislocation dynamics**

$$B\frac{\partial h}{\partial t} = \Gamma\frac{\partial^2 h}{\partial x^2} + f_p(x, h(x)) + f_a$$

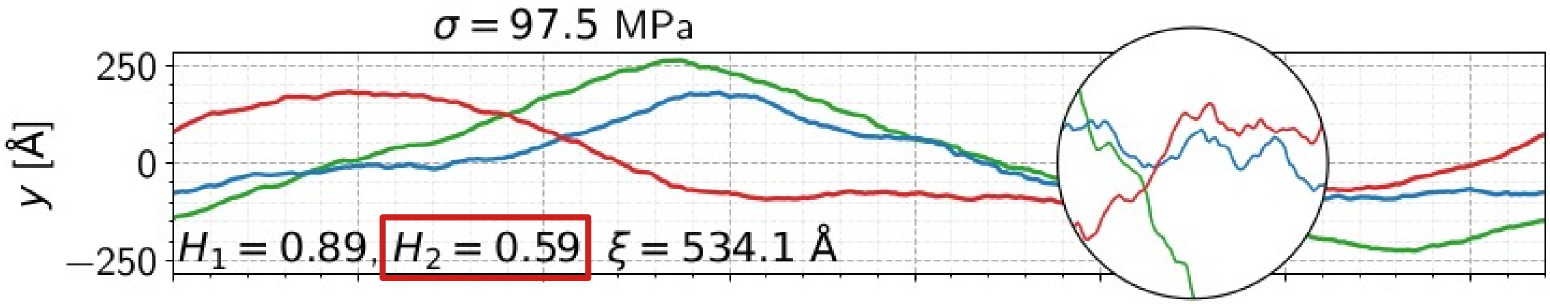
Atomistic calculations

- **Screw dislocations in Ni-Al alloy**



[Patinet, PRB 84, 174101, 2011]

- **edge dislocations in FeNiCr alloy**



[Peterffy et al. Materials Theory 4(6), 2020]

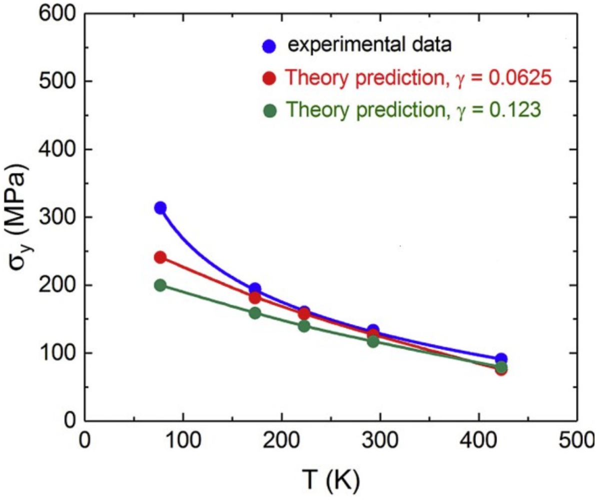
Conclusion

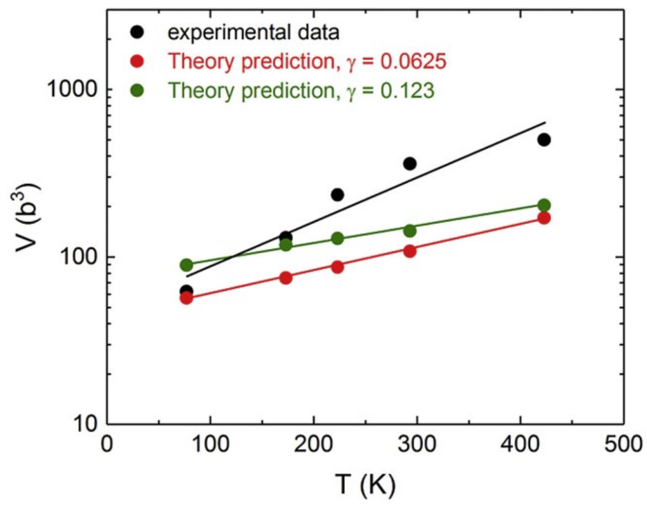
Summary

- Stress correlations influence differently dislocation of various characters
- Fixed orientations lead to different universality classes
- In real systems, we expect dislocations to align along the hard direction (edge)

Outlook

- Compare with atomistic calculations
- Role of temperature → creep





Laplanche, Guillaume, et al. "Thermal activation parameters of plastic flow reveal deformation mechanisms in the CrMnFeCoNi high-entropy alloy." Acta Materialia 143 (2018): 257-264.

Thank you for your attention

Papers

- P-A Geslin, D. Rodney, J. Mech. Phys. Sol. 153, 104479, 2021
- P-A Geslin, A. Rida, D. Rodney, J. Mech. Phys. Sol. 153, 104480, 2021
- A. Rida, E. Martinez, D. Rodney, P.A. Geslin. Phys. Rev. Mater. 6, 033605, 2022
- B. Sboui, D. Rodney, P.-A. Geslin, Acta Mater. 257, 119117, 2023
- P.-A. Geslin Computational Materials Science 232, 112624, 2024
- D. Rodney, P-A. Geslin, S. Patinet, V. Demery, A. Rosso, MSMSE 32, 035007, 2024

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