Concentrated random alloys: Interplay between dislocations and correlated stress environment

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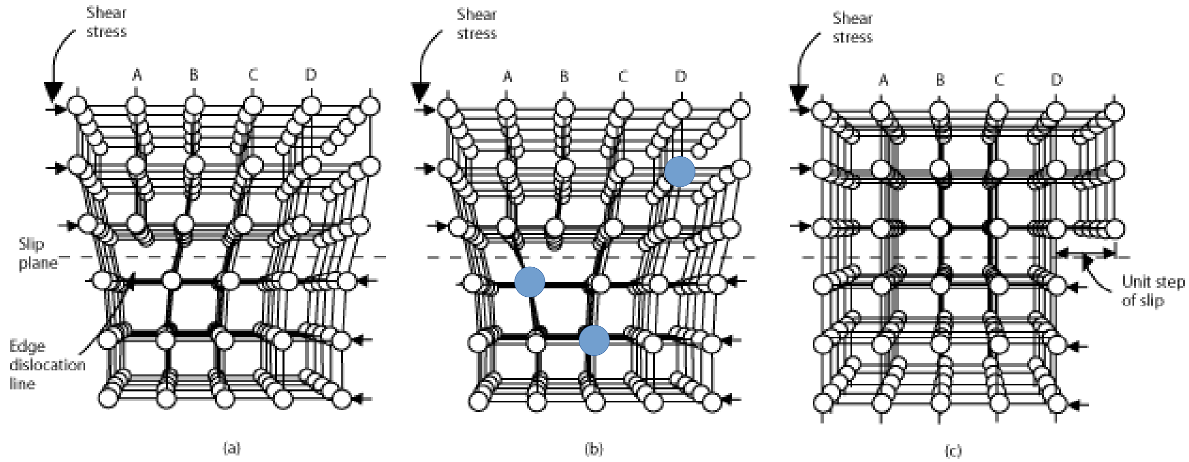
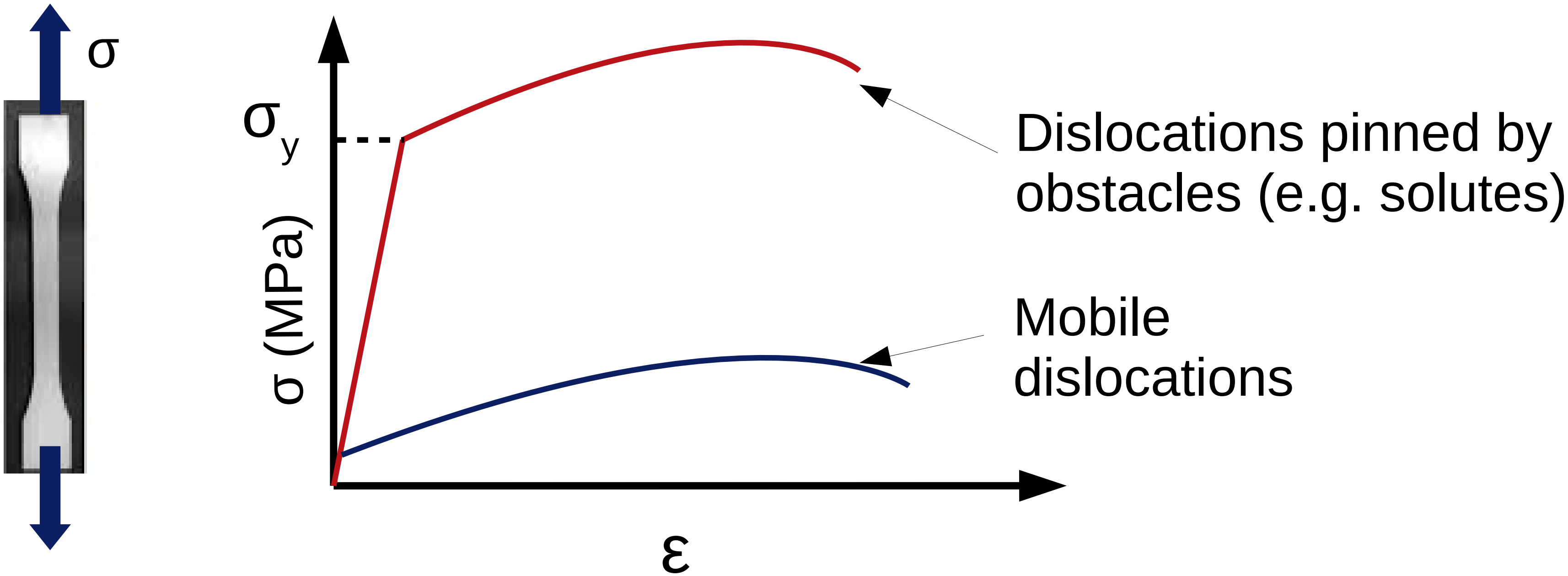
Context: plasticity of alloys

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

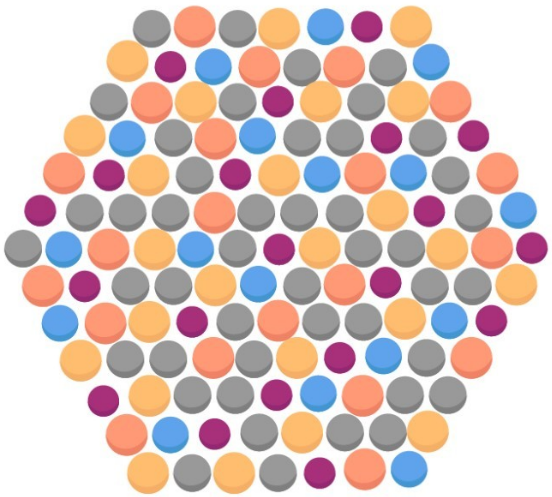


- **…that control the yield stress of the alloy**

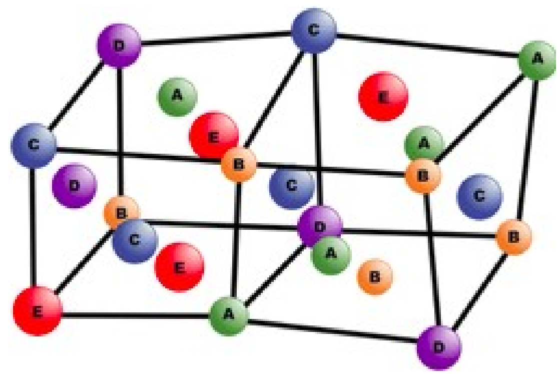


Context: solid solution strengthening

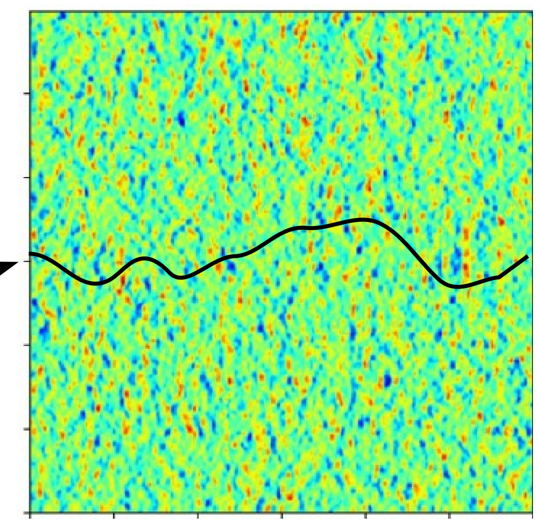
Concentrated alloy



Lattice distortions



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



$\langle u^2 \rangle$ **- is related to the yield stress of the alloy [1]**
- can be measured experimentally (XRD) [2]

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

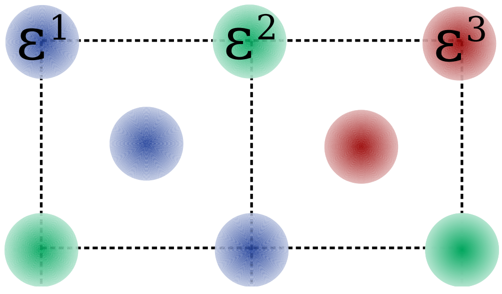
Open questions:

- **Can we predict $\langle u^2 \rangle$ and $\langle \tau^2 \rangle$ for a specific alloy ?**
- **Do these fields have spatial correlations ?**
- **How do these correlations influence dislocation depinning ?**

[1] Okamoto, et al. AIP Advances 6.12 (2016): 125008.
[2] Zhang, Yong, et al. Progress in Materials Science 61 (2014): 1-93.

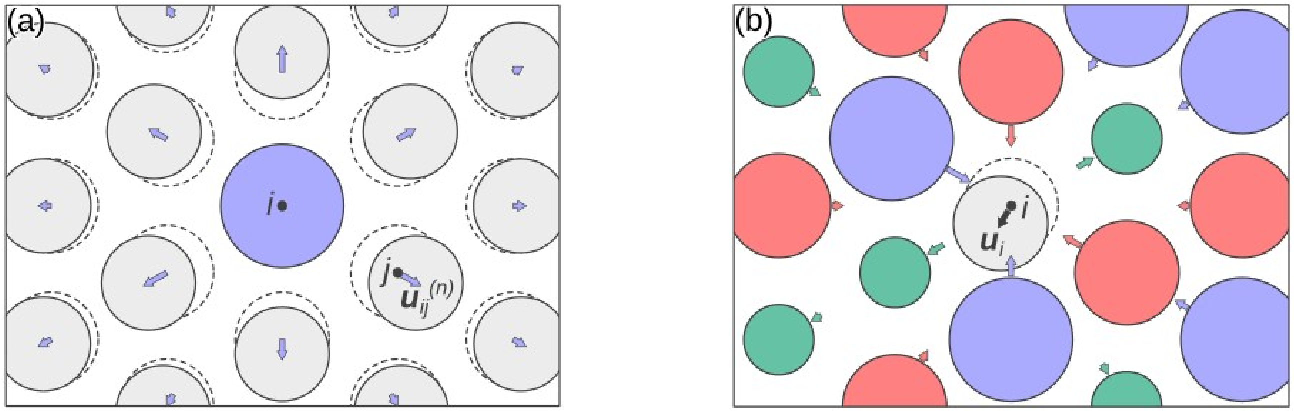
Elastic model of random alloys

- **HEA = Eshelby inclusions in an isotropic continuous medium**



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

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



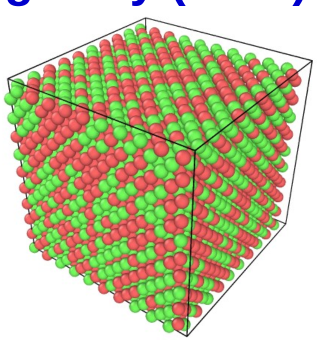
Displacements:

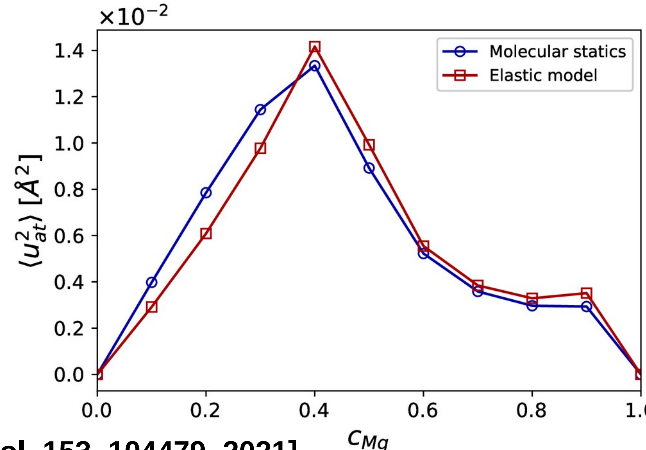
$$\boldsymbol{u}^{Eshelby}(\boldsymbol{r}) = \varepsilon \frac{v_{at}}{4\pi} \frac{1+\nu}{1-\nu} \frac{\boldsymbol{r}}{|\boldsymbol{r}|^3} \qquad \langle u^2 \rangle = \frac{25.3}{16\pi^2} \frac{v_{at} \sum_\alpha c_\alpha \varepsilon_\alpha^2}{a_{lat}} \left(\frac{1+\nu}{1-\nu} \right)^2$$

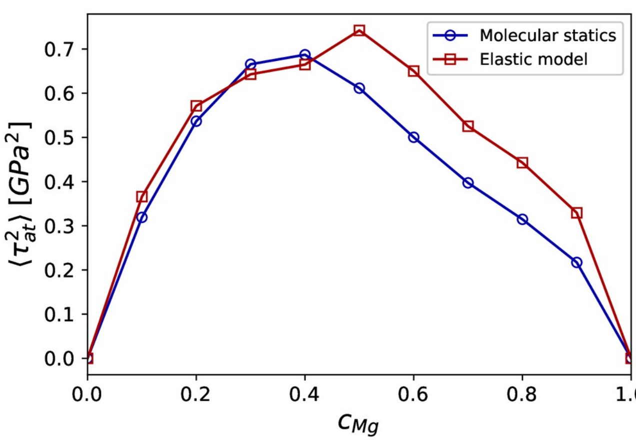
Shear stresses:

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

- **Al-Mg alloy (EAM)**



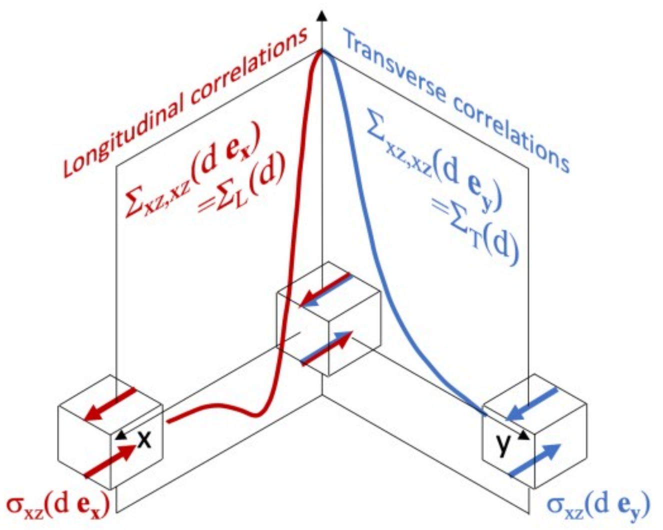




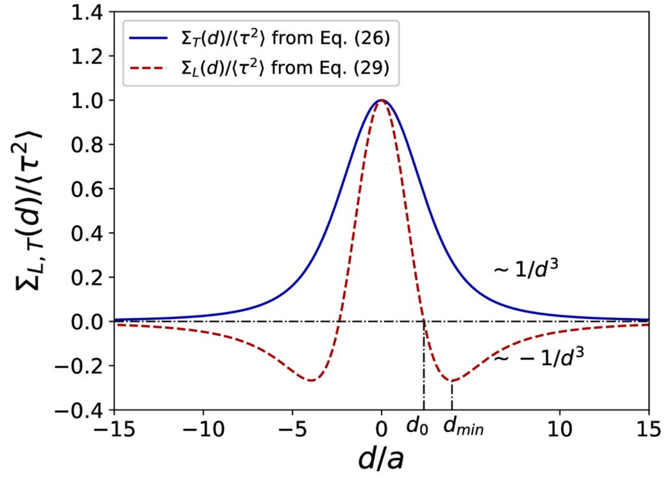
[P-A Geslin, D. Rodney, J. Mech. Phys. Sol. 153, 104479, 2021]

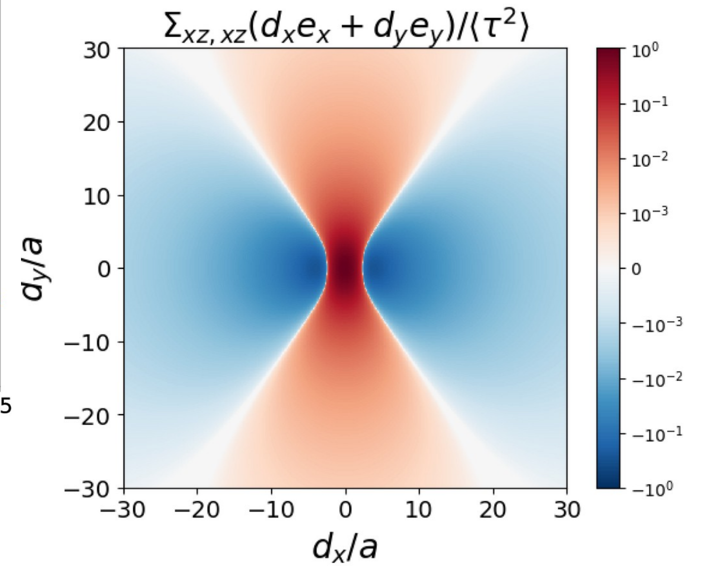
Shear stress field correlations

$$\Sigma_{ij,mn}(\boldsymbol{d}) = \langle \sigma_{ij}(\boldsymbol{r}) \overline{\sigma_{mn}(\boldsymbol{r}+\boldsymbol{d})} \rangle$$



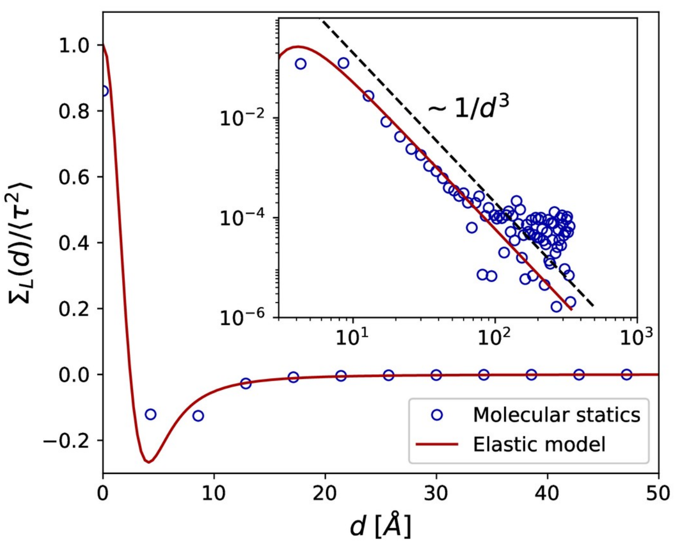
➢ Elastic model prediction

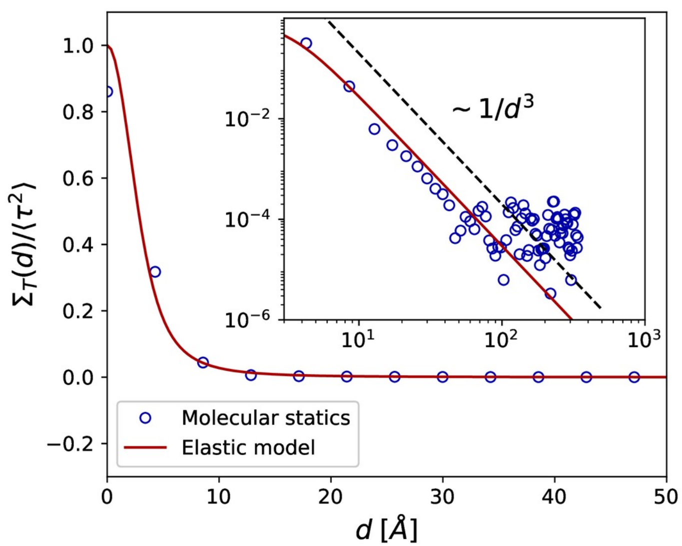


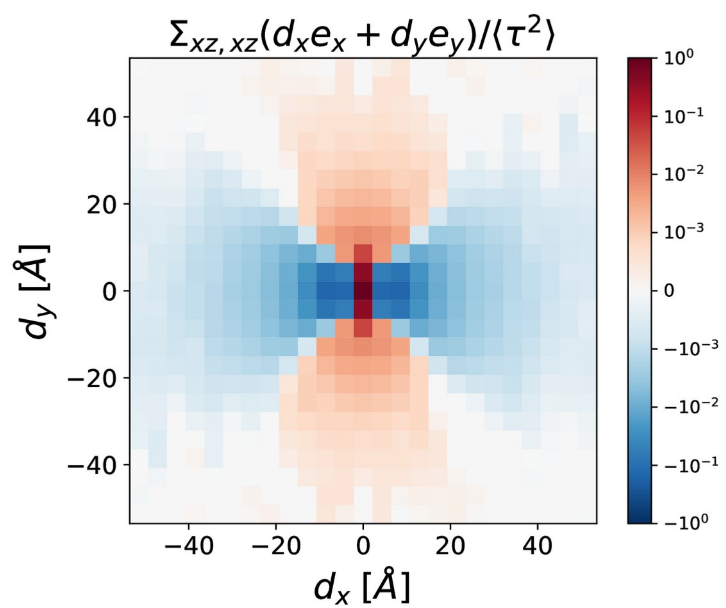


[P-A Geslin, D. Rodney, J. Mech. Phys. Sol. 153, 104480, 2021]

➢ Al-Mg system (EAM)



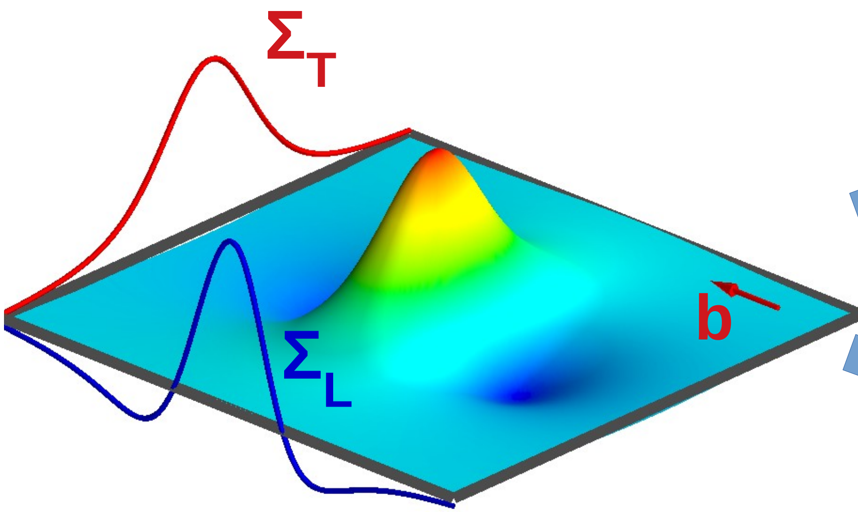


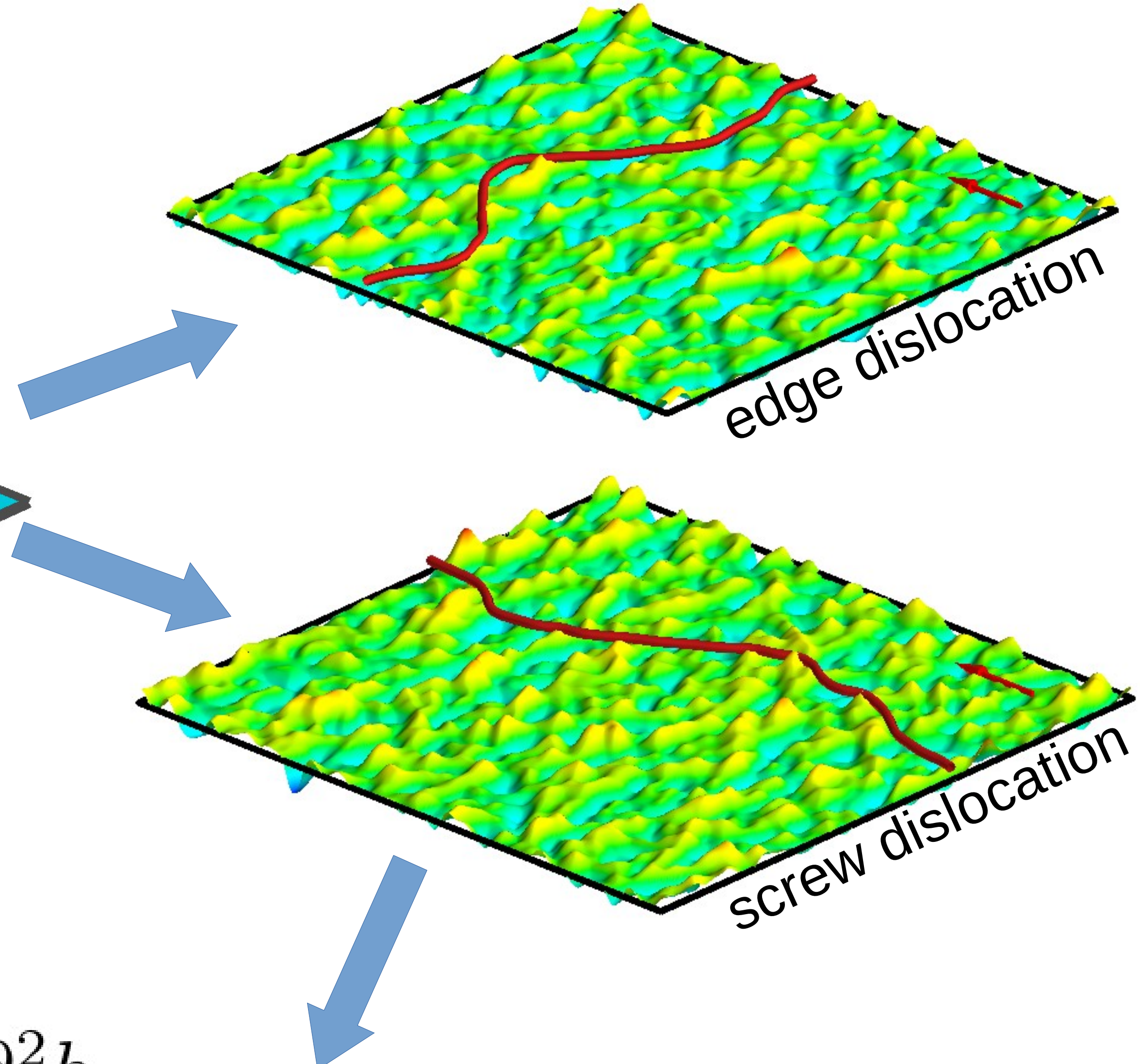


How this correlated noise affect dislocation motion ?

Dislocation depinning in correlated noise

- **Correlated noise generation**

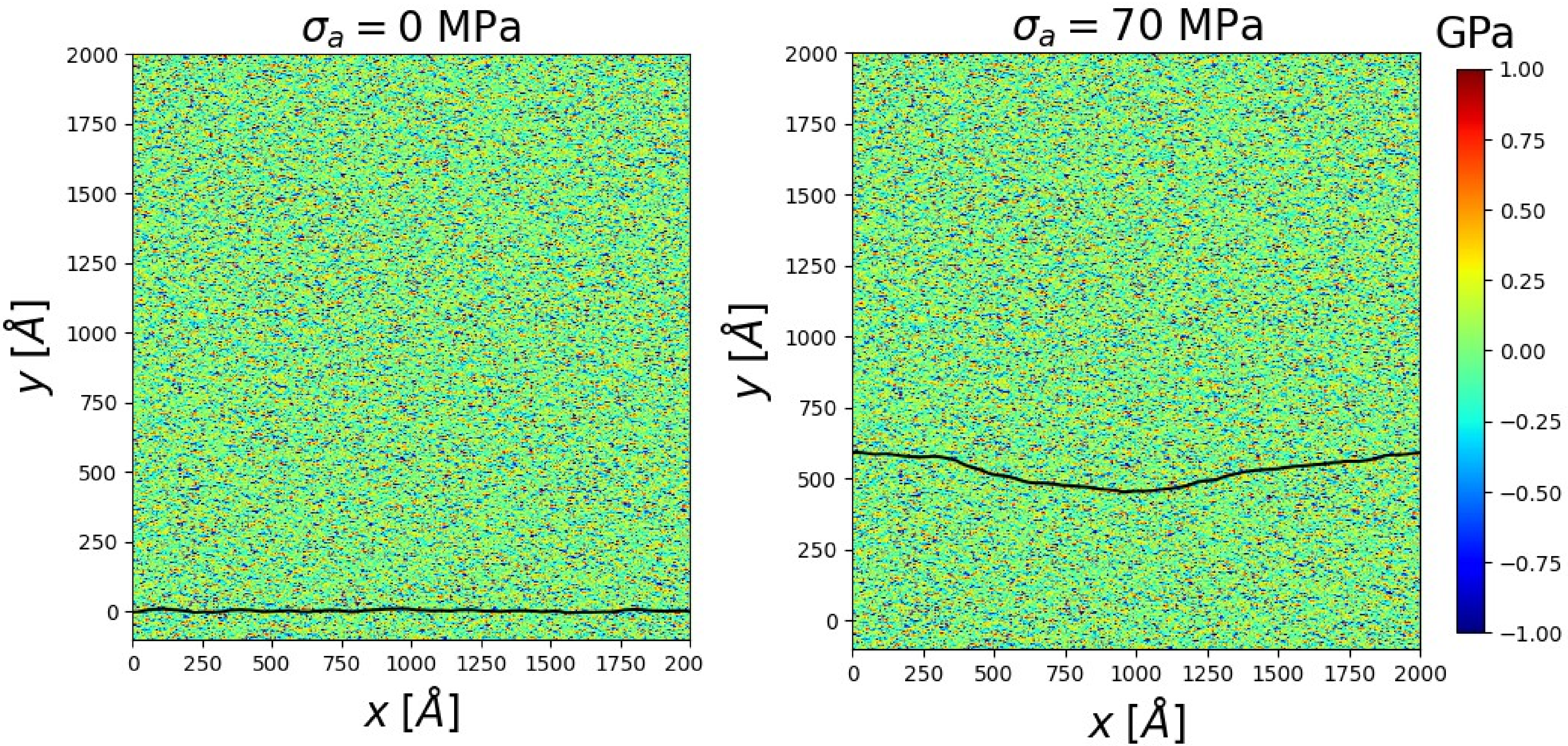




- **Dislocation dynamics**

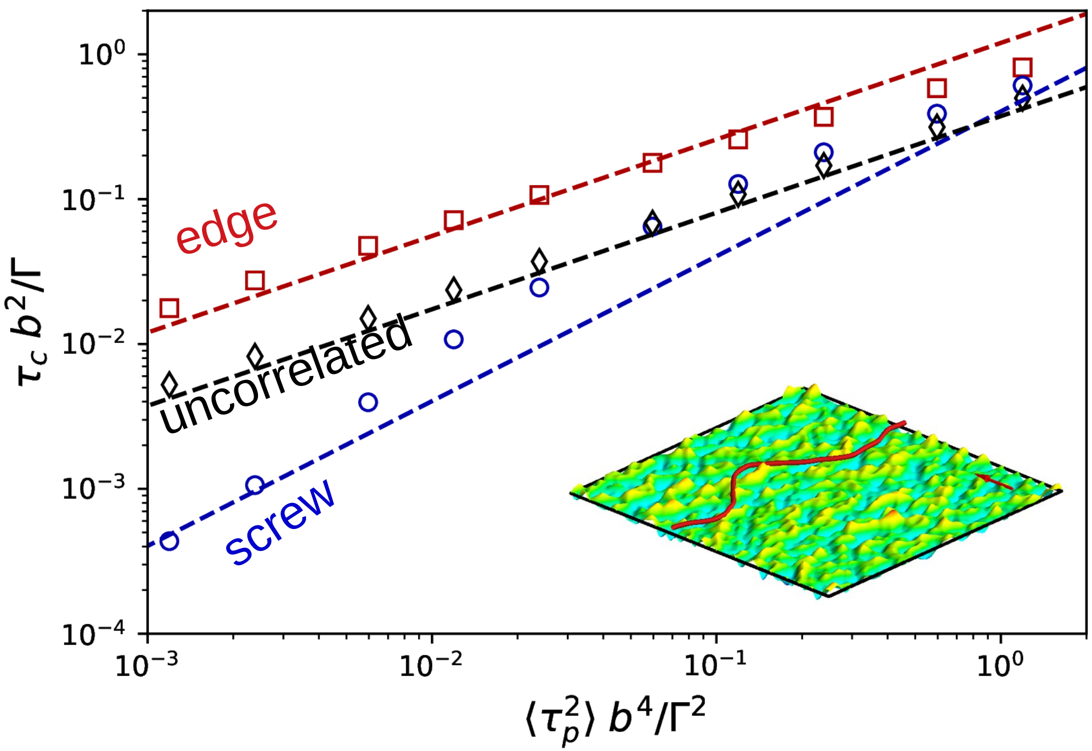
$$B\frac{\partial h}{\partial t} = -\Gamma\frac{\partial^2 h}{\partial x^2} + b(\tau_p(x, h(x)) + \tau_a)$$

Dislocation depinning in correlated noise



Dislocation depinning in correlated noise :

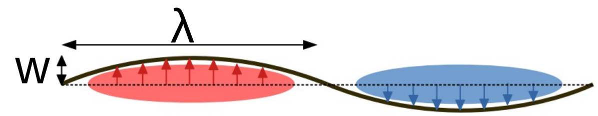
➢ **Results from dislocation dynamics model:**



- Uncorrelated noise: edge=screw and **$\tau_c \sim \langle\tau_p^2\rangle^{2/3}$**
- Edge dislocation: higher but slope close to **2/3**
- Screw dislocation: at low stress **$\tau_c \sim \langle\tau_p^2\rangle^{3/2}$**

[Larkin et al., J. Low Temp. Phys. 34, 1979]
[Zapperi, Zaiser, Mat. Sci. Eng. A 309-310, 2001]
[Zhai, Zaiser, Mat. Sci. Eng. A 740–741, 2019]

➢ **Larkin's model:**



- Only one characteristic length-scale
- Equilibrium at 0 stress gives λ_c

$$\frac{2\pi\Gamma w}{\lambda_c} = b\underbrace{\int_0^{\lambda_c} \tau_p(x,h(x))dx}$$

$$f(\lambda_c) = b\sqrt{\langle\tau_p^2\rangle \int_0^{\lambda_c}\int_0^{\lambda_c} \Sigma(x-x')dxdx'}$$

- The domain of size λ_c pins the dislocation:

$$\tau_c\lambda_c = f(\lambda_c)$$

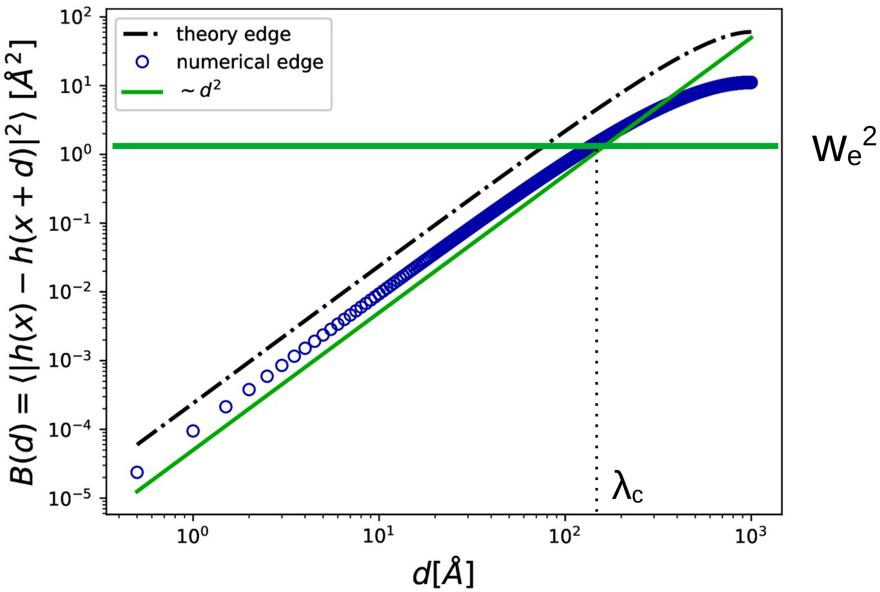
$$\tau_c^u = \left(\frac{\Delta x}{\sqrt{2\pi}}\right)^{2/3}\left(\frac{b}{\Gamma w_u}\right)^{1/3}\langle\tau_p^2\rangle^{2/3}$$

$$\tau_c^e = \left(\frac{15a}{4\sqrt{2}}\right)^{2/3}\left(\frac{b}{\Gamma w_e}\right)^{1/3}\langle\tau_p^2\rangle^{2/3}$$

$$\tau_c^s = \frac{10a^2b}{\Gamma\pi w_s}\langle\tau_p^2\rangle$$

Roughness (thanks to V. Demery, A. Rosso)

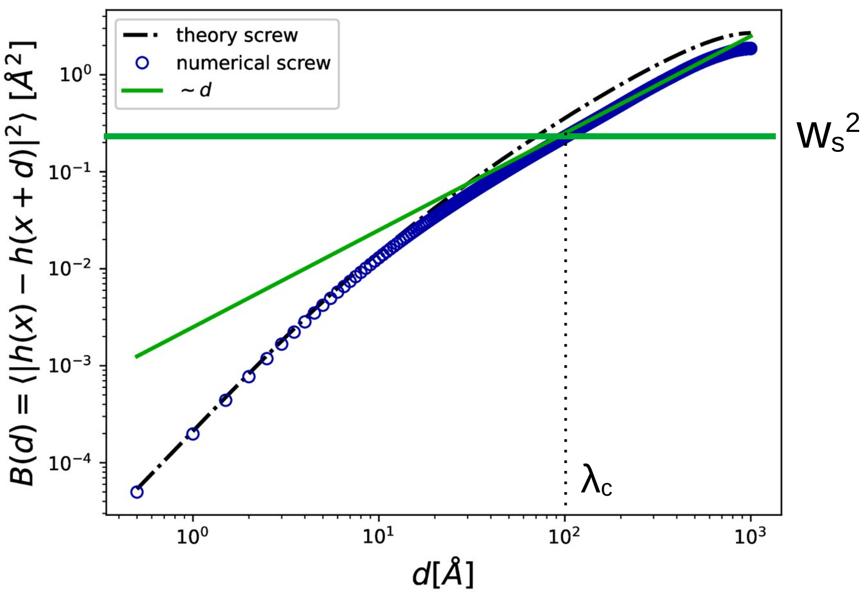
➢ **edge**



$$B_e(d) \sim \frac{d^2 L \langle \tau_p^2 \rangle}{\Gamma^2} = w_e^2$$

$$\tau_c^e \sim \frac{\langle \tau_p^2 \rangle^{2/3}}{\Gamma^{1/3}}$$

➢ **screw**

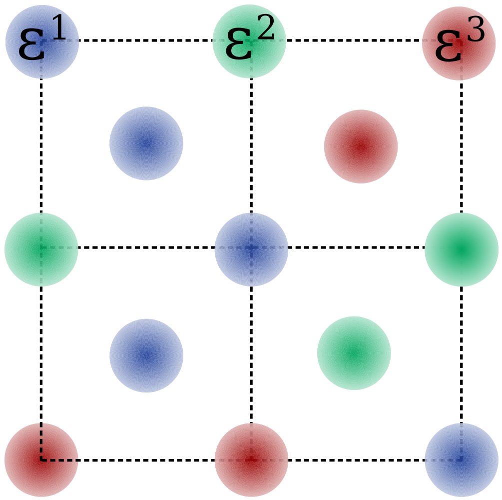


$$B_s(d) \sim \frac{d \langle \tau_p^2 \rangle}{\Gamma^2} = w_s^2$$

$$\tau_c^s \sim \frac{\langle \tau_p^2 \rangle^{3/2}}{\Gamma}$$

Most alloys are more complicated (B. Sboui)

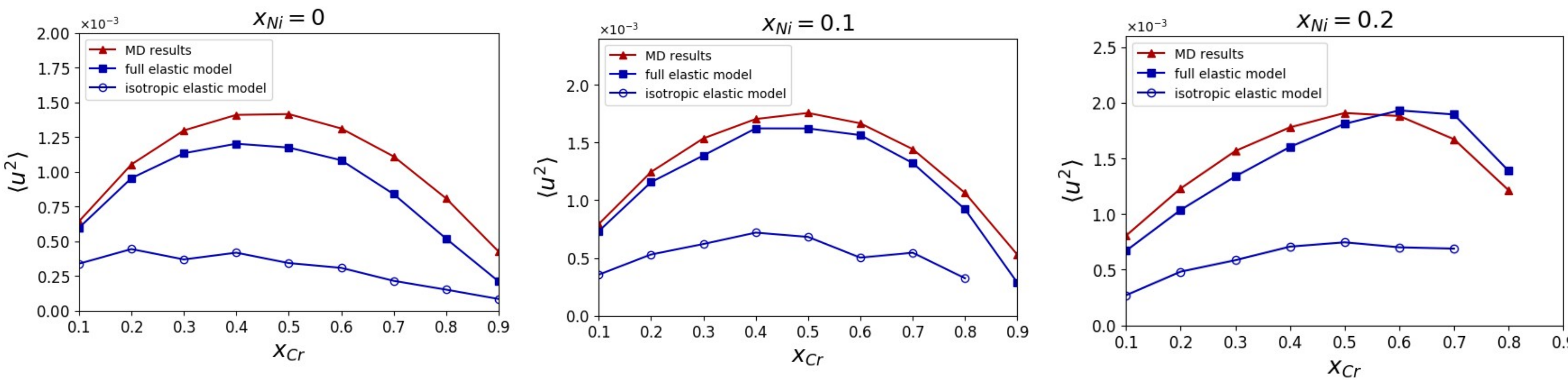
- **HEA = anisotropic Eshelby inclusions**



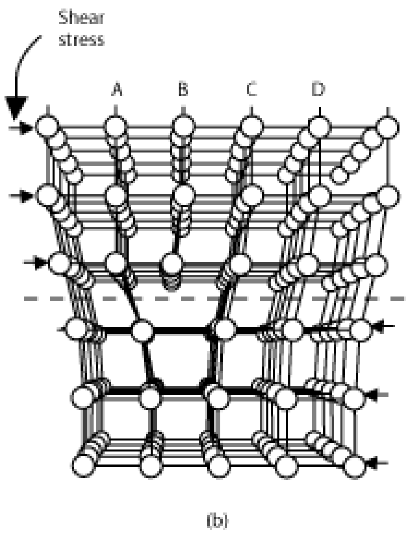
$$\bar{\bar{\varepsilon}}^{\alpha} = \begin{bmatrix} \varepsilon_{11}^{\alpha} & \varepsilon_{12}^{\alpha} & \varepsilon_{13}^{\alpha} \\ \varepsilon_{12}^{\alpha} & \varepsilon_{22}^{\alpha} & \varepsilon_{23}^{\alpha} \\ \varepsilon_{13}^{\alpha} & \varepsilon_{23}^{\alpha} & \varepsilon_{33}^{\alpha} \end{bmatrix}$$

random variable that depends on the local environment

- **Results for <u²> for Fe-Ni-Cr (FCC)**

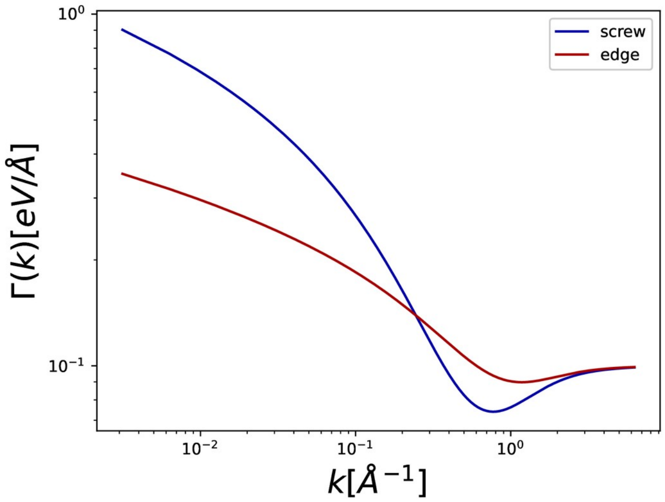


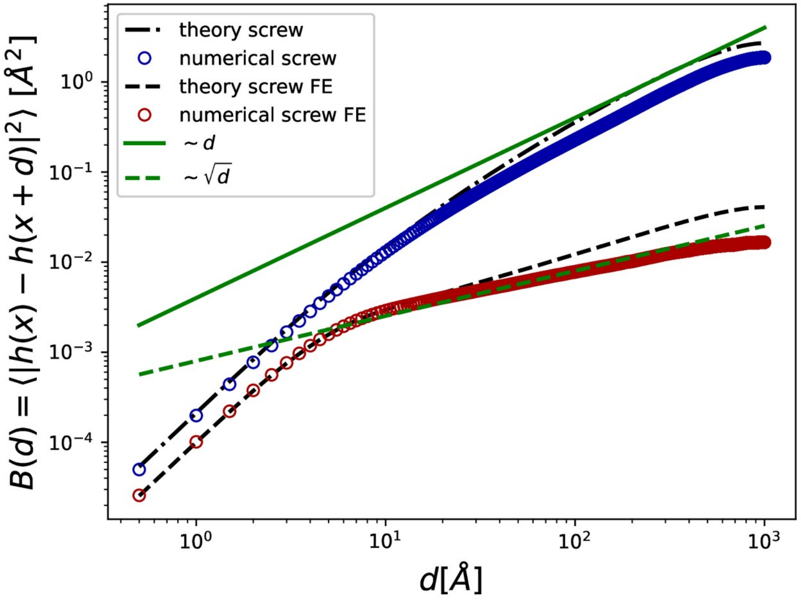
Role of long-range elasticity



σ ~ 1/r

$$\Gamma(k) \sim \frac{\mu b^2}{2\pi(1-\nu)} \ln\left(\frac{1}{k}\right)$$

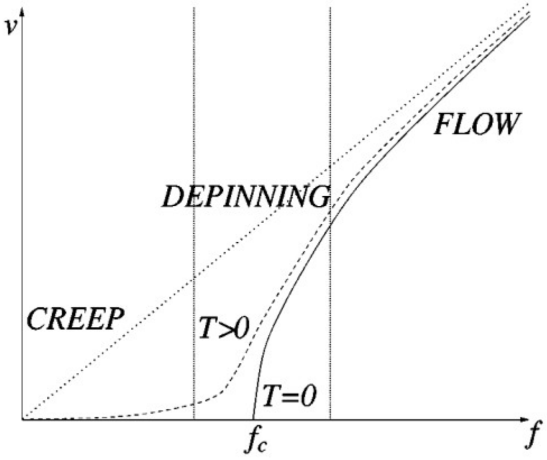




Conclusion

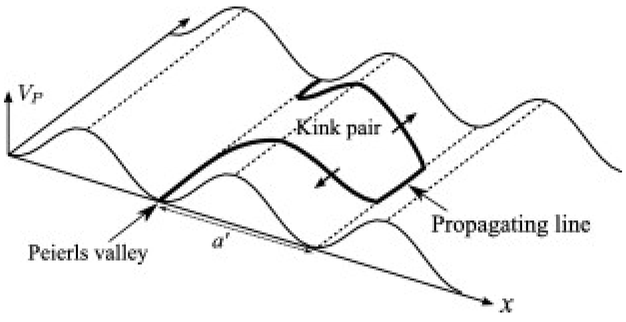
➢Outlook

➢ Exponents with long-range elasticity Γ(k) ?



➢ Add thermal noise => creep

➢ Peierls energy for screw in BCC alloys



➢Funding

➢ *Impulsion* grant from IDEXLYON (ANR-16-IDEX-005)

➢ ANR grant INSPIRA (ANR-20-CE08-0019)

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