Diffusion along dislocation cores in metals

How do atoms move in the dislocation core?

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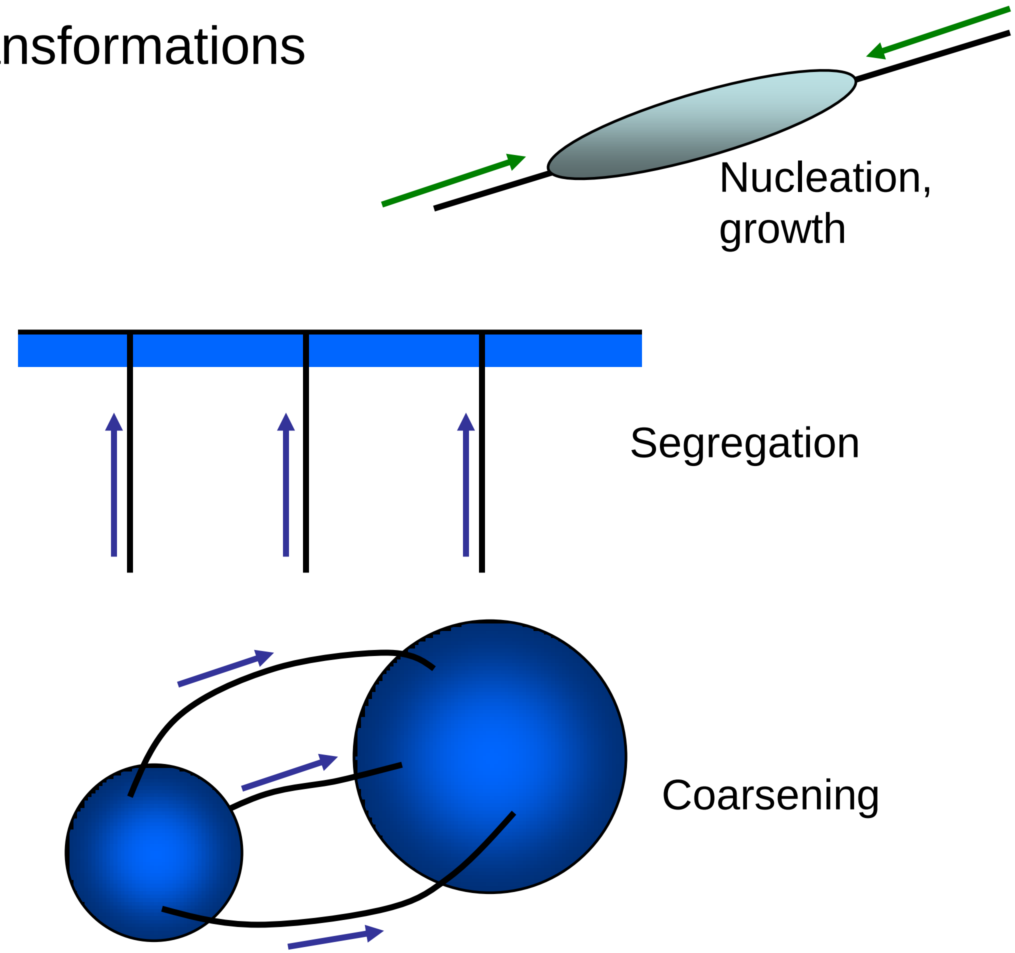
Outline

- What do we know about dislocation (“pipe”) diffusion?
  - Experimental data
  - Theory and modeling
- Diffusion along a ½<110> screw dislocation in Al
  - Methodology
  - Results
  - Do we need point defects for dislocation diffusion?

Dislocation diffusion in materials:
Why is it important?

Processes controlled/affected by dislocation diffusion:

- Precipitation and phase transformations
- Dynamic strain ageing
- Solute segregation
- Creep
- Coarsening
- Mechanical alloying
- Sintering
- Many others



Measurements of dislocation diffusion

- **Direct** measurements: from concentration profiles. $\Rightarrow P_d=\pi r_d^2 D_d$
  - Usually require radioactive isotopes
  - Based on simplified models: *a la* Fisher but with a regular arrangement of parallel dislocations (wall or network)
  - Interpretation of experimental data often problematic
  - Most of the direct measurements have been done in the 1960s-70s and summarized by Balluffi and Granato (1979). Few measurements in the 1980s-1990s; ***very*** few these days.
  - The most recent paper on dislocation self-diffusion in metals: Y. Shima et al.Mater. Trans. 43, 173 (2002), ultra-high-purity iron
  - SIMS can be used for impurity diffusion
- **Indirect methods:** from kinetics of processes
  - Internal friction
  - Dislocation climb
  - Dislocation loop shrinkage
  - Void shrinkage
  - Based on crude models with unknown parameters. Highly inaccurate

Simulations of dislocation diffusion

- Mainly calculations of vacancy formation energies and jump barriers at 0 K. Low barriers - fast diffusion
- Identification of “high-diffusivity paths”
- Correlation factors are ignored. – Big mistake!
- Quasi-1D confinement may lead to strong correlation effects (Stark, late 1980s; Qin and Murch, 1993)
- MD simulations: diffusion coefficients of vacancies, not atoms
- Only vacancies were considered in almost all studies

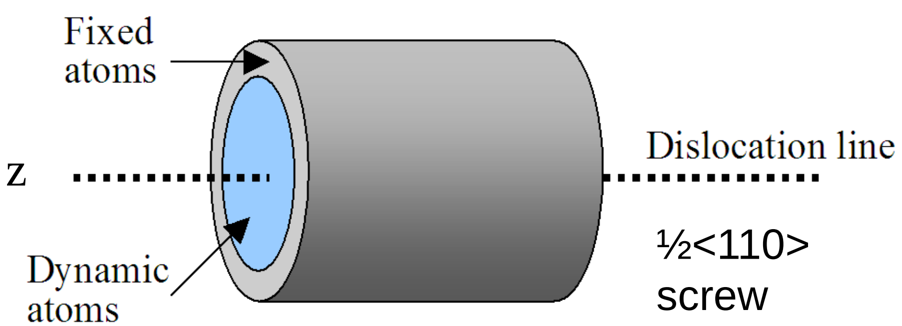
What do we know about dislocation diffusion today?

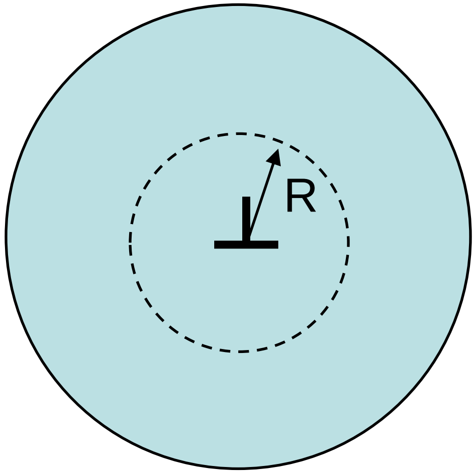
- Not much…

- $D_d >> D$; $Q_d = (0.6\text{-}0.7)Q$; both depend on the dislocation Burgers vector and character (edge/screw)
- Diffusion is *believed* to be mediated by vacancies. The actual diffusion mechanisms remain unknown
- Analogy with GB diffusion suggest a variety of possible mechanisms

Diffusion along a ½[110] screw dislocation in Al

- EAM potential for Al. Accurately reproduces c_{ij}, γ_{SF}, point defects, diffusion, etc.
- Cylindrical block with dynamic and fixed atoms (7344 total)
- Dissociation into Shockley partials in agreement with experiment
- Introduce a single defect (vacancy or interstitial), or no defect
- Run MD for 30 nanoseconds at 750-1000 K (T_m= 1042 K)
- MSD of atoms for 3-7 ns: $\overline{D}(R) = \langle z^2 \rangle / 2t$
- Correction for equilibrium defect concentration



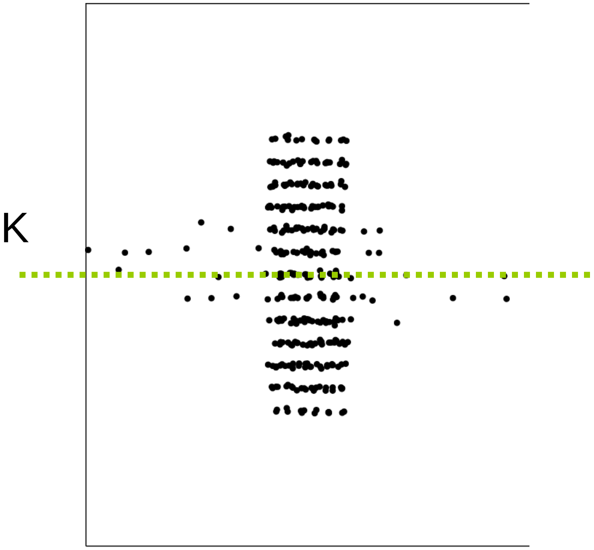


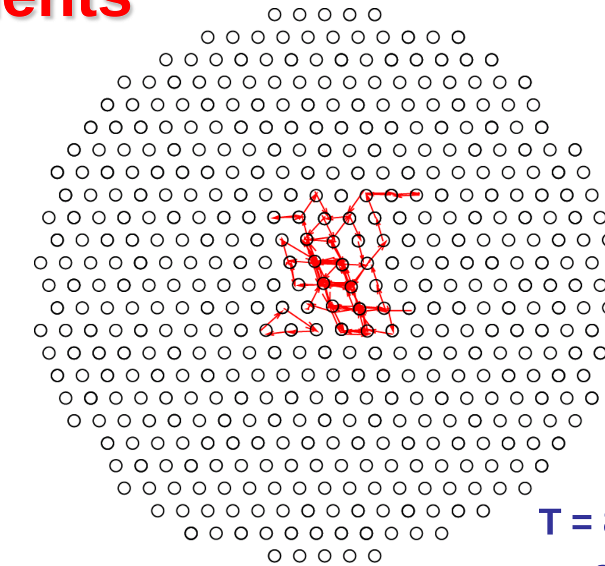
Output: $\overline{D}(R)$

Mean-squared displacements

1000 K

5 ns



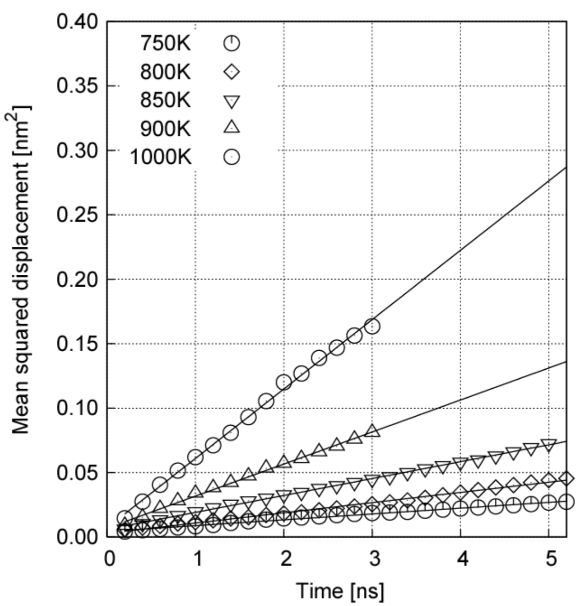


T = 800 K

t = 3 ns

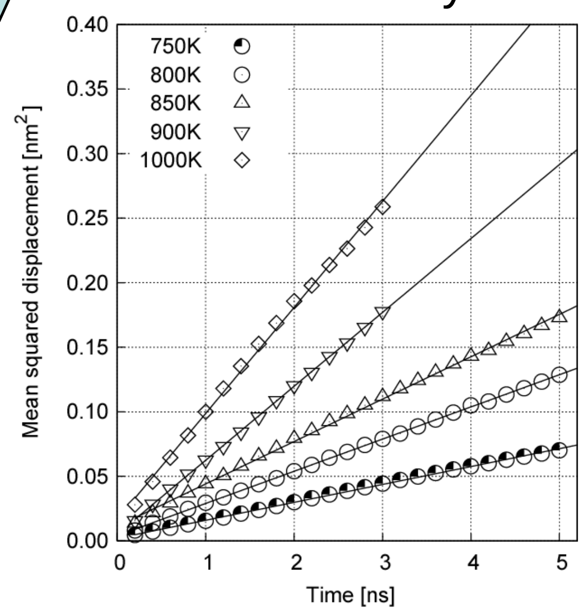
$$\overline{D}(R)$$

Intrinsic!!!



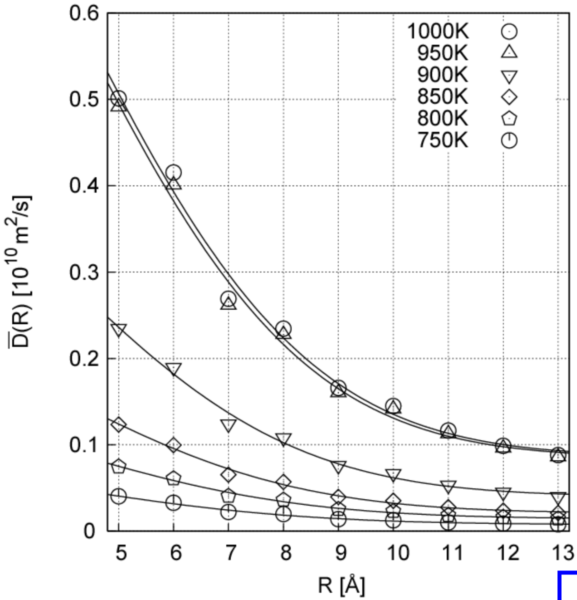
R=0.7 nm

With a vacancy

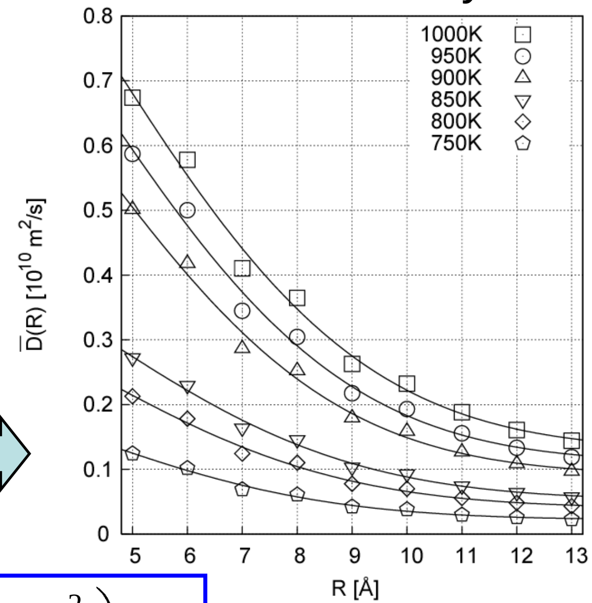


How to find the dislocation diffusivity

Intrinsic



With a vacancy



$$\boxed{\overline{D}(R) = A\exp\left(-\frac{R^2}{r_d^2}\right) + B}$$

$D^I_d \approx A/e;\ r_d$

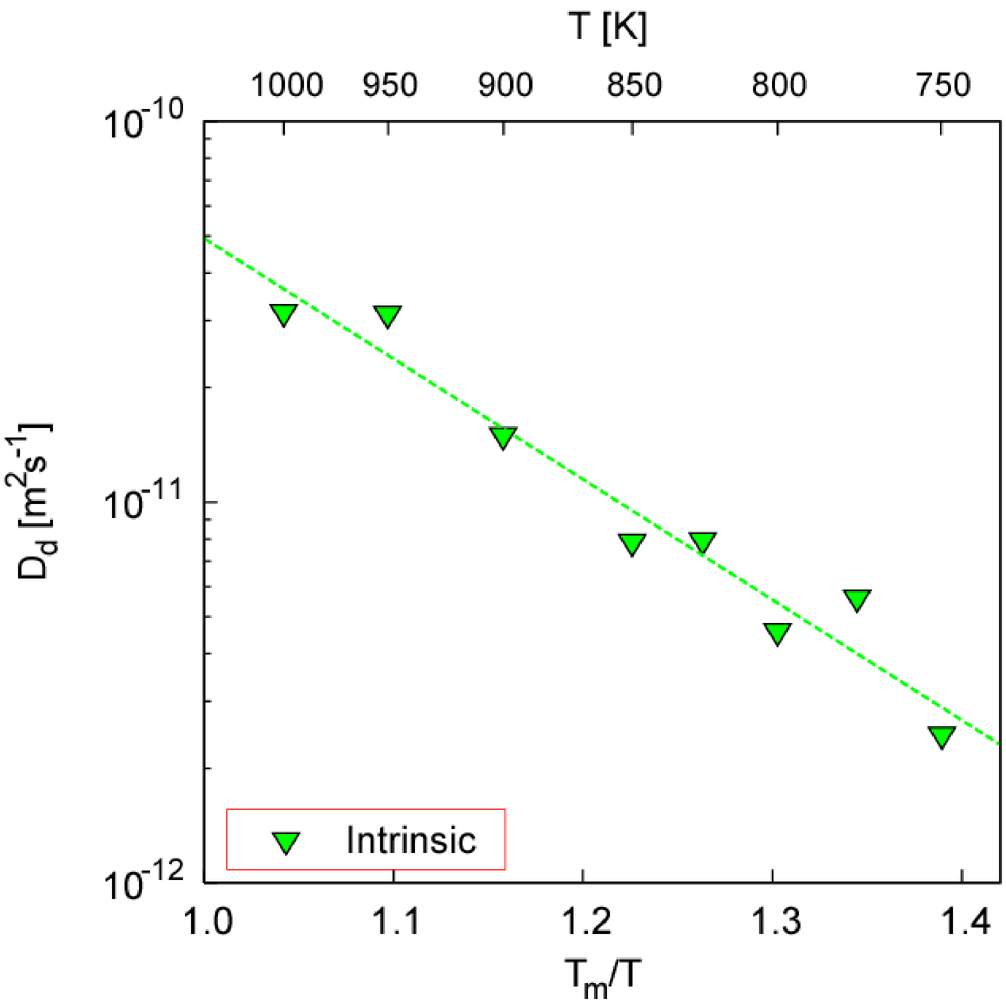
$D_d^{raw} \approx A/e;\ r_d$

$$D_d = D_d^I + N_v\left(D_d^{raw} - D_d^I\right)$$

$$N_v = \sum_{i=1}^{n} \exp\left(-\frac{E_{vi}}{kT}\right)$$

Similar equation for interstitials

Intrinsic dislocation diffusivity



E_d = 0.65 eV

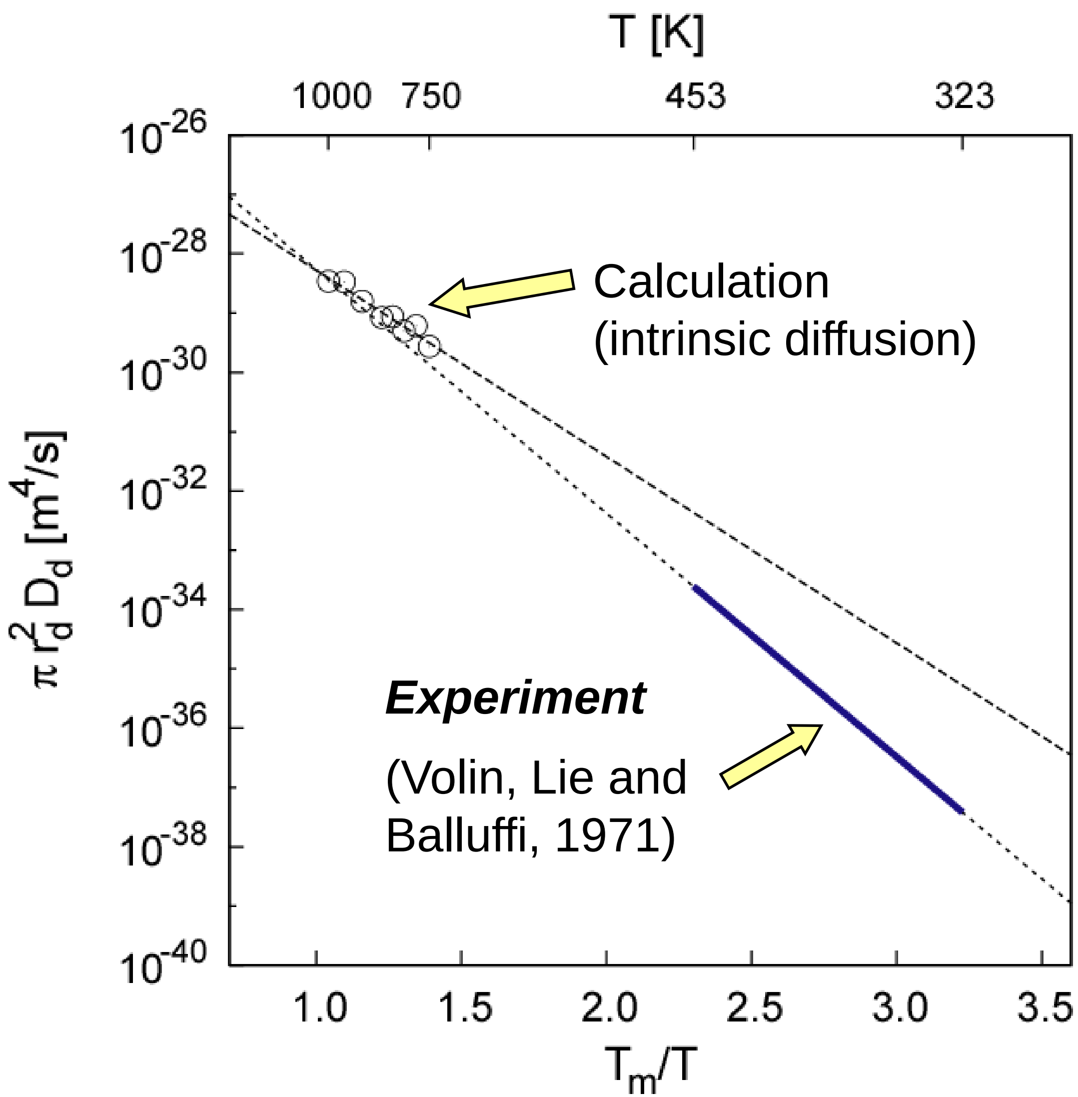
D_{d0} = 7.24×10^{-8} m^2/s

r_d = 0.59 nm

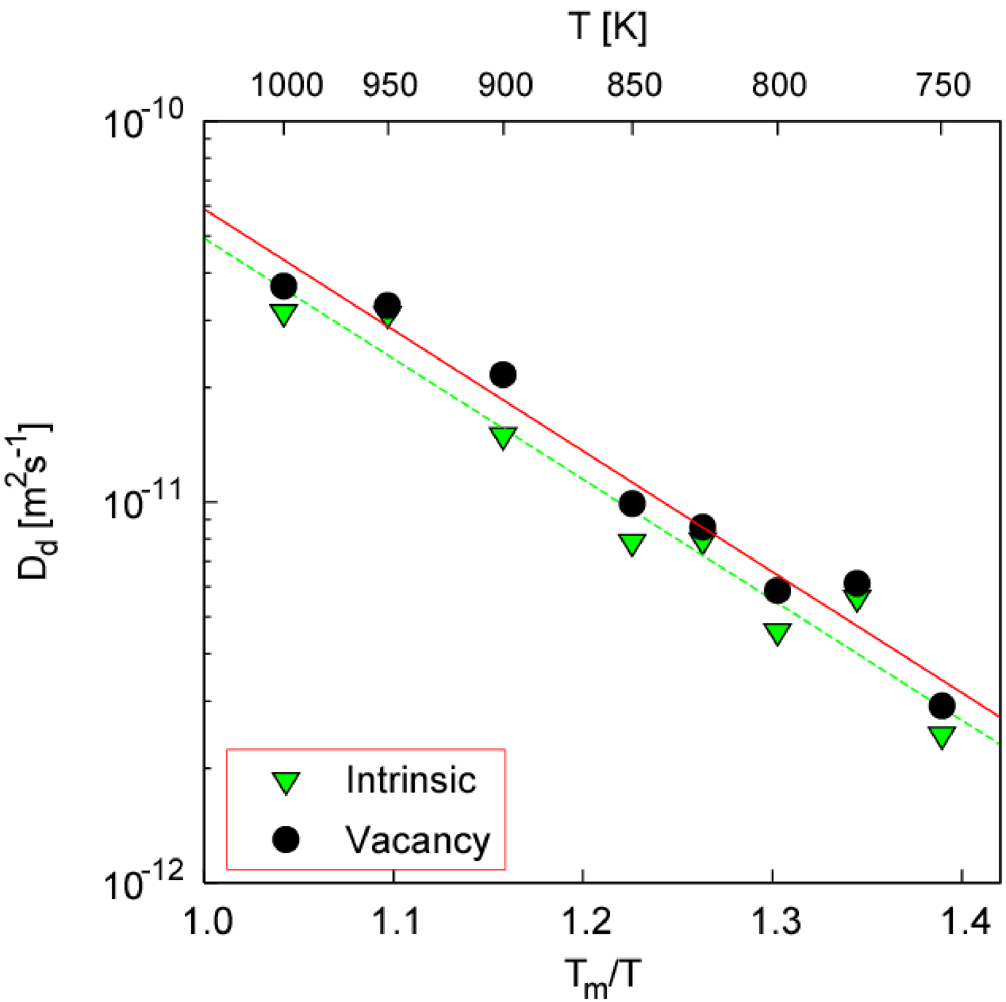
E = 1.32 eV

E_d/E = 0.49

Comparison with experiment



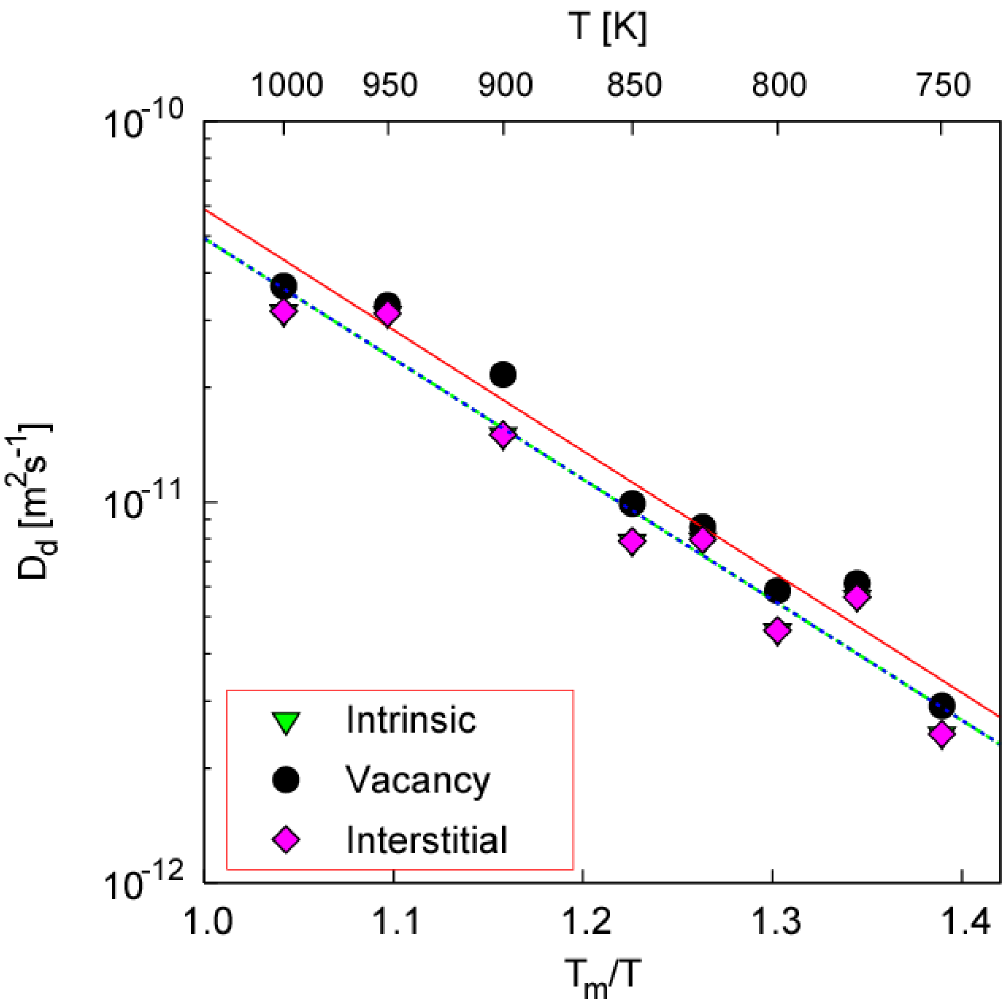
Contribution of vacancy diffusion



$E_d = 0.66$ eV

The vacancy contribution is relatively small

Contribution of interstitial diffusion



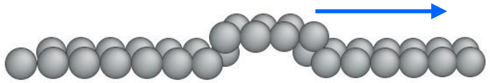
E_d = 0.65 eV

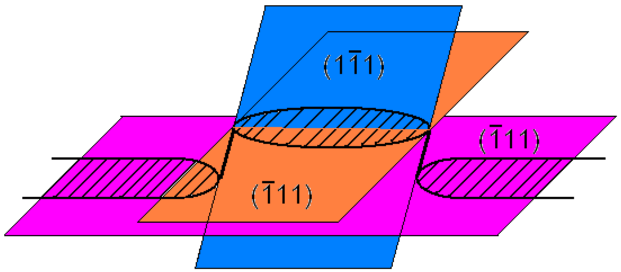
The interstitial contribution is negligible

The intrinsic diffusion dominates!

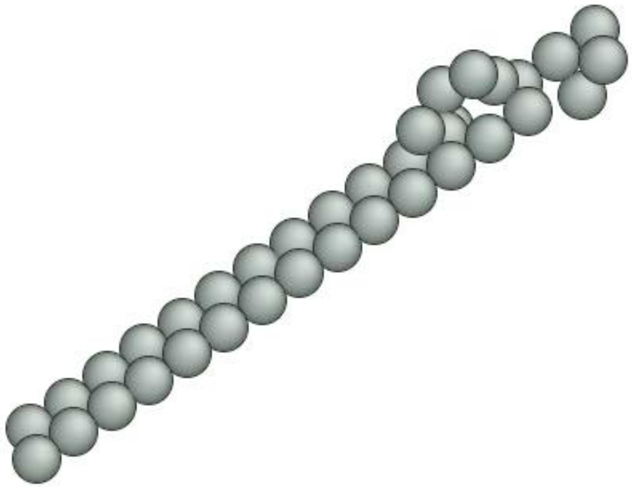
What is the intrinsic mechanism?

- The dislocation line moves around the average position due to thermal fluctuations
- The motion occurs by the nucleation and spreading of double-jogs $\Rightarrow$ shuffling of atoms
- This thermal motion has a stochastic component which gives rise to diffusion
- Perfect sliding would translate entire rows $\Rightarrow$ zero correlation factor
- Need to understand more details





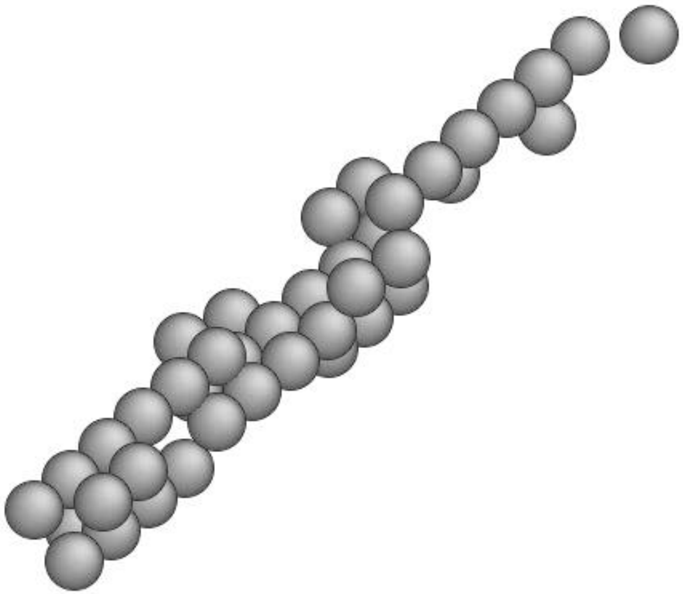
Dislocation with a vacancy



- The vacancy is wandering around the core
- The vacancy is not absorbed by the core
- Due to the thermal motion, the dislocation easily breaks away from the vacancy
- Does the vacancy induce the jog formation?

Visualization by potential energy

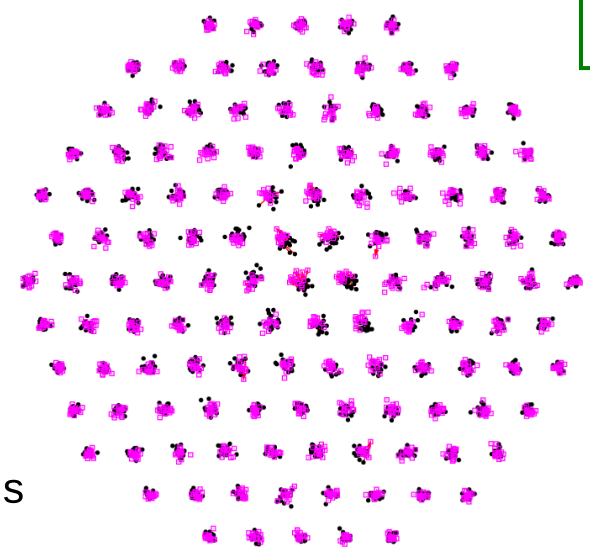
Dislocation without point defects



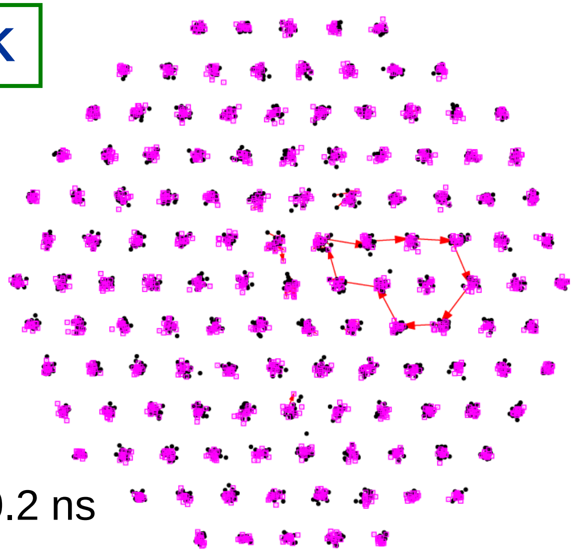
Still observe jog formation and thermal motion

Vacancy excursions: Intrinsic case

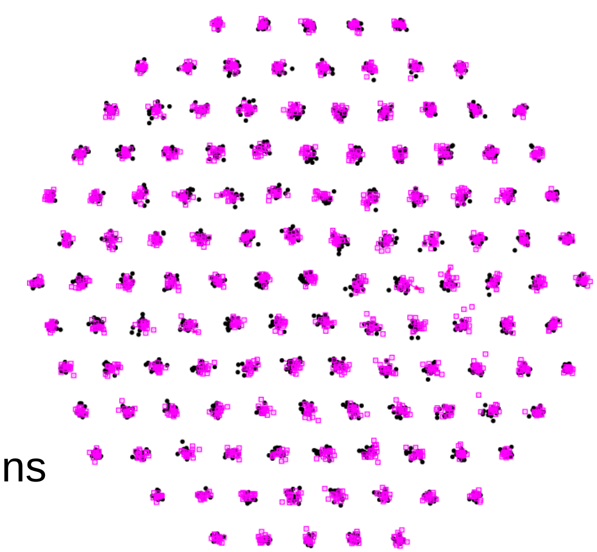
T = 900 K



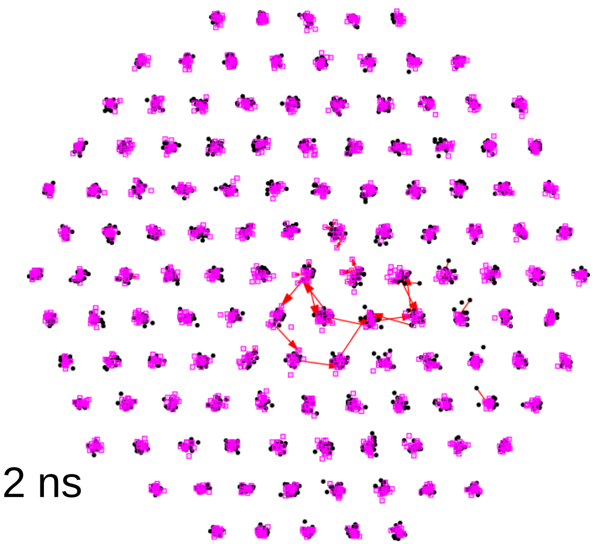
0 ns



0.2 ns



0 ns



0.2 ns

Ongoing and future work

- What exactly happens in the core during the extrinsic diffusion process?
- Extension to edge and mixed dislocations

  [preliminary result: no significant intrinsic diffusion in edge dislocations]
- Instead of Al, try a metal with a low stacking fault energy
- Extension to the Al-Li
- If the intrinsic diffusion is confirmed, we may need to reconsider the role of point defects in dislocation diffusion