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 $\frac{1}{2}<110>$ screw dislocation in Al
  - Methodology
  - Results
  - Do we need point defects for dislocation diffusion?
Processes controlled/affected by dislocation diffusion:

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

Dislocation diffusion in materials: Why is it important?
Measurements of dislocation diffusion

- **Direct** measurements: from concentration profiles. \( P_d = \pi r_d^2 D_d \)
  - 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.
  - 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...

- $D_d >> D$; $Q_d = (0.6-0.7)Q$; 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 $\frac{1}{2}[110]$ screw dislocation in Al

- EAM potential for Al. Accurately reproduces $c_{ij}$, $\gamma_{SF}$, 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: $\overline{D}(R)$
Intrinsic!!!

\[ T = 800 \text{ K} \]
\[ t = 3 \text{ ns} \]

Mean-squared displacements

\[ \overline{D}(R) \]

$R = 0.7 \text{ nm}$

With a vacancy

NIST Diffusion Workshop, May 2007
How to find the dislocation diffusivity

**Intrinsic**

\[ \bar{D}(R) = A \exp \left( -\frac{R^2}{r_d^2} \right) + B \]

\[ D_d = D_d^I + N_v \exp \left( -\frac{E_{vi}}{kT} \right) \]

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

**With a vacancy**

\[ \bar{D}(R) \]

\[ D_d^{\text{raw}} \approx A/e; r_d \]

Similar equation for interstitials

*NIST Diffusion Workshop, May 2007*
Intrinsic dislocation diffusivity

\[ E_d = 0.65 \text{ eV} \]
\[ D_{d0} = 7.24 \times 10^{-8} \text{ m}^2/\text{s} \]
\[ r_d = 0.59 \text{ nm} \]
\[ E = 1.32 \text{ eV} \]
\[ E_d/E = 0.49 \]
Comparison with experiment

Experiment
(Volin, Lie and Balluffi, 1971)

Calculation
(intrinsic diffusion)
Contribution of vacancy diffusion

The vacancy contribution is relatively small

E_d = 0.66 eV

The vacancy contribution is relatively small
Contribution of interstitial diffusion

The interstitial contribution is negligible.

The intrinsic diffusion dominates!

$E_d = 0.65$ eV

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 ⇒ shuffling of atoms.
- This thermal motion has a stochastic component which gives rise to diffusion.
- Perfect sliding would translate entire rows ⇒ 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
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