Atomistic investigation of dislocation assisted C migration in Dark Etching Regions

Tigany Zarrouk*

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Motivation

- Carbon redistribution and plastic deformation are thought to be fundamental mechanisms behind DER formation.
- Differing mechanisms of dislocation-driven carbon migration have been suggested, but no consensus.
- Atomistic modelling necessary to elucidate how dislocations could move carbon; thus clarifying potential mechanisms of DER formation.

Aims

To answer the questions:

- How do dislocations assist carbon migration?
- How are dislocations influenced by carbon on atomistic scale?
  - How does carbon affect kink-pair nucleation/migration?
  - How fast do the dislocations move in carbon environment?
  - What dislocation structures are found with dislocation movement?

*tigany.zarrouk@skf.com

Methods

Tight Binding

- Tight binding is an approximation to DFT.
- Overlaps between atomic orbitals are key parameters.
- Parameters can be fitted to experimental data.
- $\mathcal{O}(N^3)$, but much smaller prefactor compared to DFT.

Line Tension Model

- Line Tension model approximates energy along core dislocation dislocation line.
- Parameters derived from atomistics: Peierls barrier (ΔE_{P}), K, ΔE_{C}.
- Defined as

$E^{\mathrm{LT}} = \frac{K}{2}\sum_j (P_j + P_{j+1})^2 + \sum_j E_{\mathrm{P}}(\mathbf{P}_j) +$

[1] Itakura, M., *et al.*, Acta Materialia (2013).

Kinetic Monte Carlo

- kMC simulations model the movement of dislocations on much larger timescales than atomistics.
- Propogation of dislocation line segments are treated as rare events with particular rates and mechanisms depending on local environment.
- Rates for each of the mechanism are derived from atomistic calculations.
- One can find dislocation velocity as a function of stress and temperature.

Summary of Methods

- Tight-binding simulations to determine influence of carbon on dislocations and for line-tension model constants.
- Line tension model of dislocation to acquire stress-dependent kink-pair formation energies.

- Kinetic Monte Carlo model of dislocations in carbon environment to ascertain behaviour of dislocations in carbon environment.

Plan

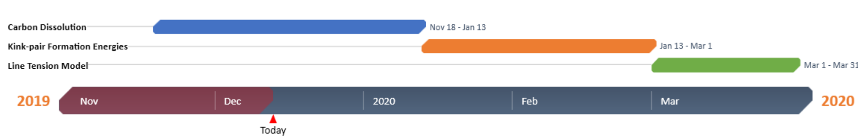
<u>Tight-binding:</u>

1. C/defect solution energies
   (a) In perfect lattice
   (b) With dislocation
2. Dislocation core reconstruction with C
3. Constants for line tension model.

<u>Line-tension model:</u>

1. Kink-pair formation energies
   (a) Without C
   (b) With C in different interstitial sites
   (c) Under stress
2. kMC transition rates

Gantt Chart



Summary

- Dislocation-assisted carbon migration thought to be fundamental mechanism behind DER formation.
- No consensus on which mechanism is correct, if it is at all the case.
- Simulations can give insight into how dislocations interact with carbon, thus elucidating potential mechanism.
- Tight-binding can be used to model energetics of carbon and dislocations and constants for line-tension model.
- Line-tension model can obtain kink-pair formation energies for kMC model.
- kMC model can be used to see dislocation behaviour on longer length and timescales, allowing for us to elucidate mechanisms of dislocation-assisted carbon migration.

References