**Atomistic simulations of pipe diffusion in bcc iron**

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**Pipe diffusion**

3D bulk diffusion (before being trapped by the dislocation)

(Quasi-)1D pipe diffusion along the dislocation line

**Motivation**

- Recent experimental findings [1] confirmed higher diffusivity in the core of dislocations (i.e., pipe diffusion) compared to bulk.
- Some models use pipe diffusion to explain dynamic strain aging in metallic alloys.
- Long time scale simulations with Atomistic Kinetic Monte Carlo (AKMC), in turn, may provide additional insights on the pipe diffusion phenomena.
- Effective diffusivity and activation energy, which can be eventually compared to experiments.
- The cross section of the dislocation pipe (assumed to be a disc or radius \(b\)) in Ref. [1].
- \(b\) behavior in the core of dislocations in Fe is a timely issue in metallurgy [2], considering that C-dislocation interactions play a major role in the mechanical properties of steels.

**Simulation protocol**

The simulations consisted of two steps:

1. The energy barriers at \(T=0\) K for C jumps in the core (defined as a region where \(R < 4b\) ~ 0.25 nm) of an edge and a screw dislocation in bcc Fe were calculated using the NEB method as implemented in the LAMMPS package and the Fe-C EAM potential presented in Ref. [4].
2. Using a catalog containing the transitions and corresponding energy barriers, a number of C trajectories in the core of an edge and a screw dislocation were simulated by AKMC employing a rigid lattice, where each site represented an energy minimum corresponding to the C atom occupying an interstitial site in the bcc Fe lattice.

**Results**

**Energy barriers**

- About 2,000 transitions in the region defined as the dislocation core were investigated with LAMMPS-NEB.
- Energy barriers within a wide range: 0.14-1.55 eV (0.82 eV in the bulk, according to the EAM potential).

**Simulations**

- 1,000 C trajectories with up to 10,000,000 C jumps
- Temperatures considered in the simulations: 300-1000 K

For \(T < 400\) K (edge) and \(T < 700\) K (screw) no actual diffusion is observed along the dislocation line: we observe that the C atom visits repeatedly a few sites separated by low energy barriers, which form a superbasin (see the next figures).

Above these temperatures, C diffusion along the dislocation line is observed but the C atom is also more likely to escape the dislocation core (i.e., bulk diffusion becomes more important than pipe diffusion).

**Conclusions and work in progress**

- Counterintuitively, the analysis of the energy barriers in the core of dislocations and some preliminary AKMC simulations suggest that dislocations may act as traps rather than fast diffusivity channels for C atoms in bcc Fe.
- Nevertheless, the simple AKMC algorithm used in this work is not appropriate to address the low barrier problem represented in Figs. 3, 4, and 5, which is particularly important at low \(T\).
- A solution to be implemented in the next step is the mean rate method proposed by Ref. [5], where slow (diffusive) transitions are treated separately from the fast transitions inside the superbasin.