Atomistic simulations of pipe diffusion in bcc iron

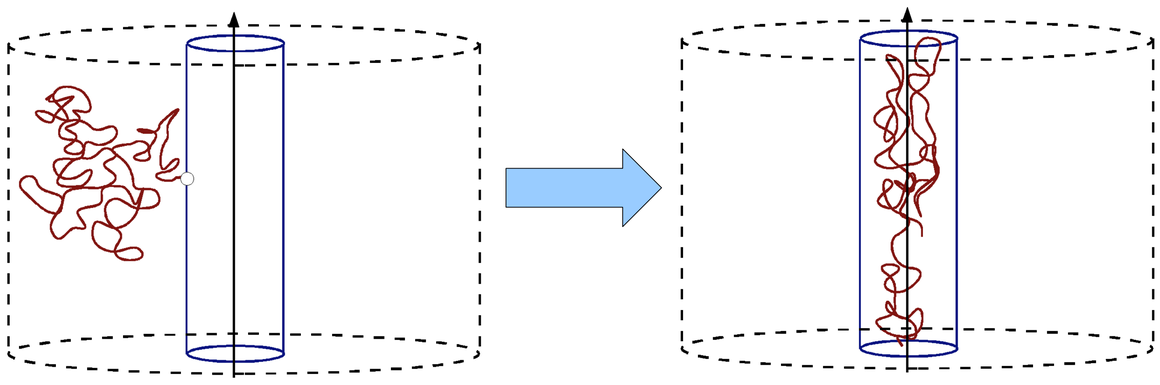
Roberto Gomes de Aguiar Veiga[1,2], Michel Perez[1], Charlotte Becquart[3], and Christophe Domain[4]

(1) Laboratoire MATEIS, INSA Lyon, Université de Lyon, UMR CNRS 5510, Villeurbanne, France.
(2) Departamento de Engenharia Metalurgica e de Materiais, Escola Politécnica, Universidade de São Paulo, São Paulo, Brazil.
(3) Unité Matériaux et Transformations (UMET), EM2VM, Ecole Nationale Supérieure de Chimie de Lille, UMR CNRS 8207, Villeneuve d'Ascq, France.
(4) Recherche et Développement, Matériaux et Mécanique des Composants, EDF, EM2VM, Les Renardières, Moret sur Loing, France.

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
- Simulation data are scarce and obtained by MD up to a few nanoseconds [2,3]
- 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])
- C 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 < 4*b* ~ 1 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)

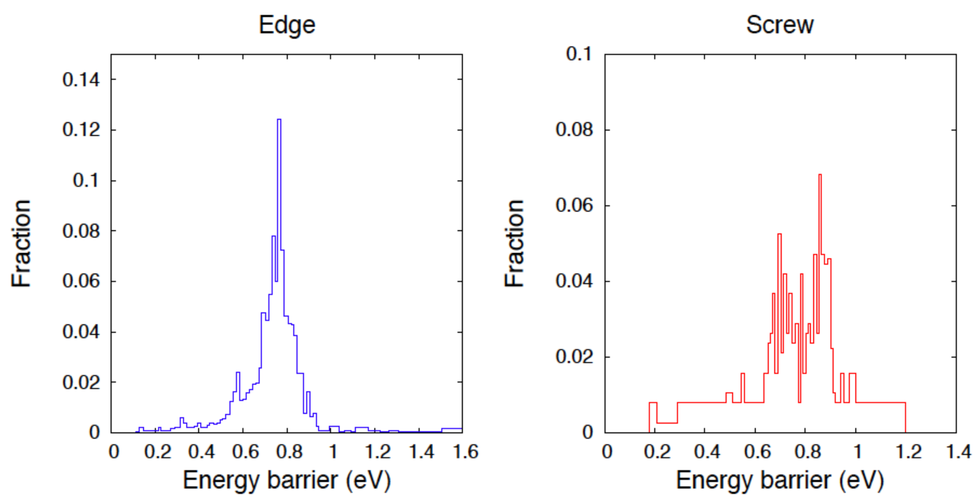


Fig. 2 - Energy barrier distribution in the regions defined as the core (R < 4*b* ~ 1 nm) of an edge and a screw dislocation.

AKMC 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)

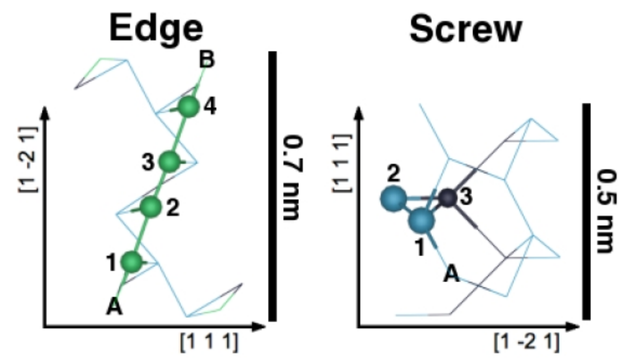


Fig. 3 - Minimum energy positions where a C atom can be found within a distance of *b* ~ 0.25 nm from the dislocation line. Spheres represent sites that taken together form a superbasin where the C atom is trapped. C-dislocation binding energies: 0.6-0.7 eV (green); 0.4-0.5 eV (blue); and 0.3-0.4 eV (black). **A** and **B** are the sites through which the C atom escapes the superbasin.

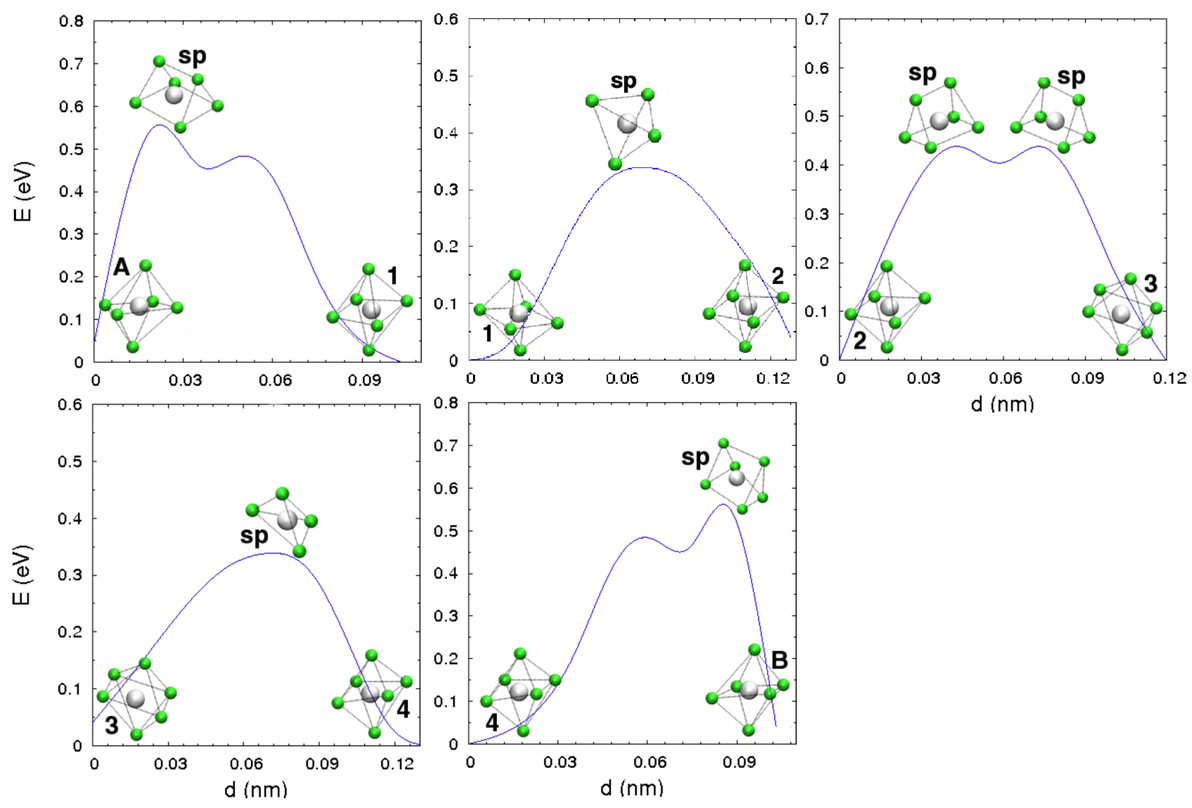


Fig. 4 - Minimum energy paths connecting the local minima shown in Fig. 3 in the core of an edge dislocation. White balls represent C atoms; green balls, Fe atoms.

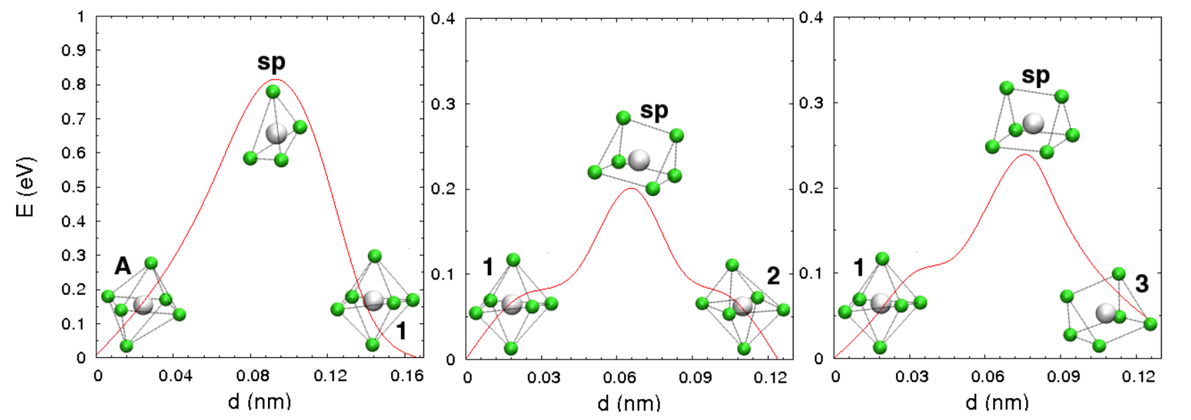


Fig. 5 - Minimum energy paths connecting the local minima shown in Fig. 3 in the core of a screw dislocation. White balls represent C atoms; green balls, Fe atoms.

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

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