Effect of the stress field of dislocations on carbon diffusion

Modelling the effect of the stress field of dislocations on carbon diffusion in α-iron

Coupling Molecular Dynamcs and Atomic Kinetic Monte-Carlo

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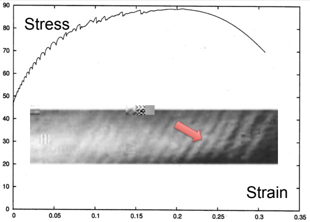
Context and challenges

General objective : Dynamic and static aging



- Portevin - Le Chatelier effect (Lüders banding)
- poorly understood (physical metallurgy challenge) !

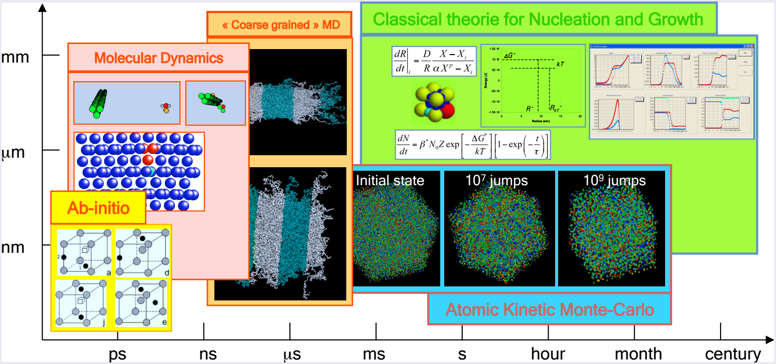
Short term objective : static ageing

How the stress field of a dislocation affects carbon diffusion

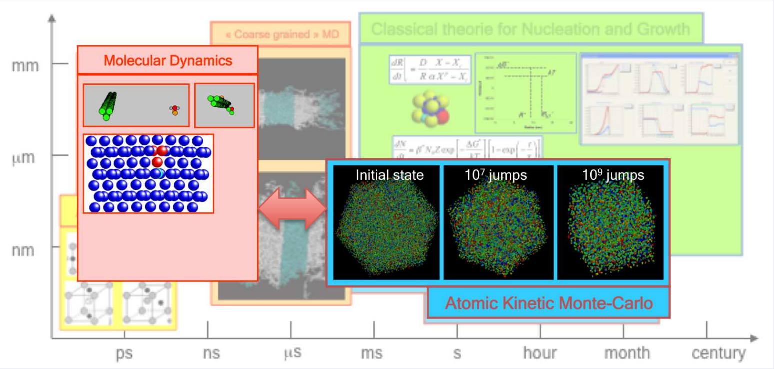
1. far from the dislocation line (low/moderate stress),
2. and right in the dislocation core (high stress) ?

Outline...

From first principles to classical nucleation and growth theory

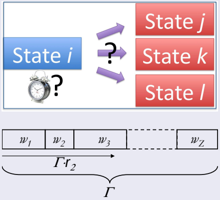


From first principles to classical nucleation and growth theory



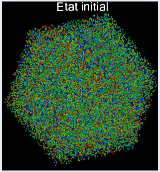
Atomic Kinetic Monte-Carlo

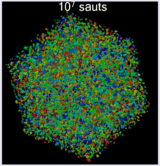
Principle

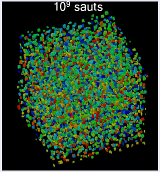


- Transition frequency from $i \rightarrow j$:
  $w_j^i = w_0 \exp\left(\frac{-\Delta E_{ij}}{kT}\right) \quad w_0 \approx 10^{14}$ Hz
- Residence time i
   $r_1 \rightarrow \tau_R = -\frac{\ln r_1}{\sum_j w_j}$
- Choice of a particular transition  r_2

Example : precipitation from a supersaturated solid solution





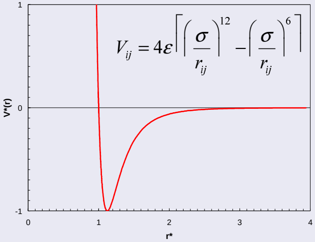


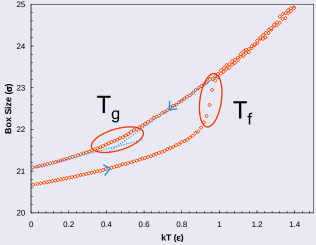
Molecular dynamics

Principle

- Newton's law $m_i \frac{d\mathbf{v}}{dt} = \mathbf{f_i}$
- Pair interaction : $\mathbf{f_i} = \sum_j \mathbf{f_{ij}} = \sum_j \mathbf{grad}\, V_{ij}$
- Thermodynamic ensembles : NVE, NVT, NPT...

Example : Fusion and glass transition





Taking out the best of two techniques

Atomic Kinetic Monte-Carlo

- Large timescale ☺
- Fixed lattice, no stress ☹

Molecular Dynamics

- Short timescale (1 ps !) ☹
- Free lattice, Stress ☺

How to couple both methods ?

- Kinetic Monte-Carlo → kinetics (needs for ΔE_{ij})
- Molecular Statics → ΔE_{ij}
- Molecular Dynamics → Deformation, stress

Applications

- uniform stress (Snoek relaxation)
- non-uniform stress (dislocation)
- non-uniform stress, lattice change (precipitation)

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Applications

- uniform stress (Snoek relaxation) [*Comp. Mat. Sc.* **43** (2008)]
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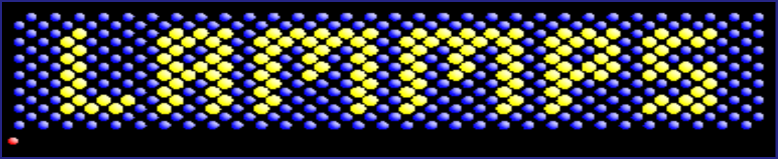
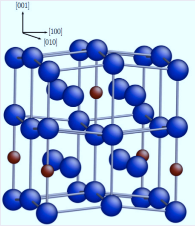
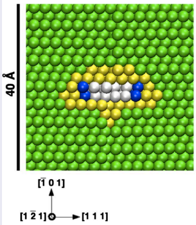
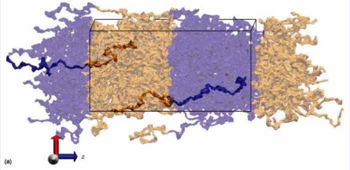
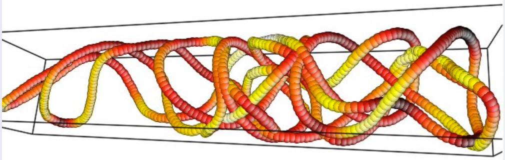
The Molecular Dynamics/Statics software...







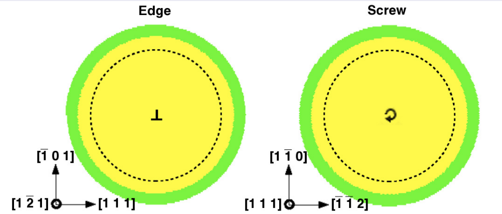




Computational model

Molecular statics simulation box

- Cylinder (radius : 150 Å)
- Dislocations → anisotropic elasticity theory
- Outer shell (atoms kept fixed)
- PBC along dislocation line only
- Octahedral and tetrahedral sites mapped
  Positions in the core not included !



An Fe-C potential [*Comp. Mat. Sc.* **40** (2007)]

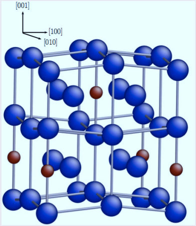
Eam (embedded atom method) potential

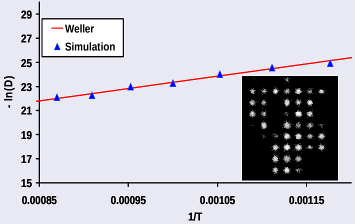
- Pair interaction AND electronic density

$$E_{tot} = \frac{1}{2}\sum_i \sum_{j\neq i} \Phi_{ij}(\mathbf{r}_{ij}) + \sum_i F_i\left(\sum_{j\neq i} \rho(\mathbf{r}_{ij})\right)$$

- Validated on two configurations : C in octa and tetra site

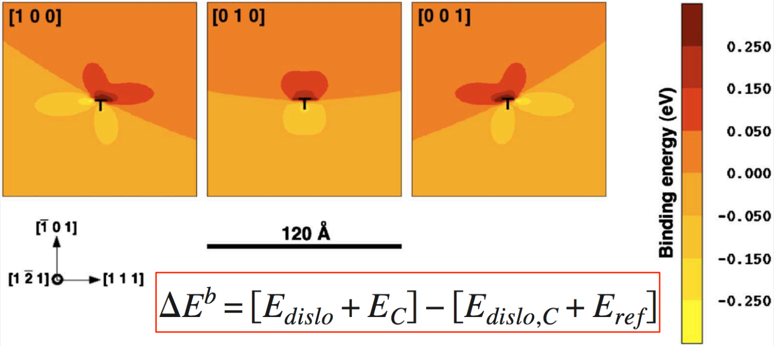
Validation of the potential : from solid solution to carbides





Binding energies

Example of the edge dislocation



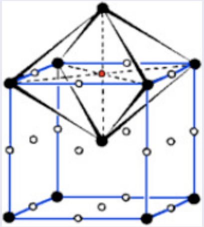
$$\Delta E^b = [E_{dislo} + E_C] - [E_{dislo,C} + E_{ref}]$$

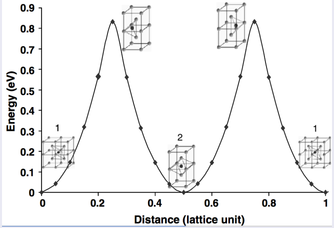
- $E_b > 0 \rightarrow$ attraction
- Right in the core $E_b = 0.66$ eV

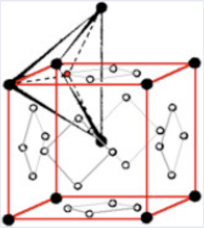
Migration energies

Minimum energy path

- Transition : octa (energy minimum) → tetra (saddle point) → octa (energy minimum)
- Carbon @ octa → full energy minimization
- Otherwise → carbon to relax only on the plane ⊥ migration coordinate (octa–to–octa line)







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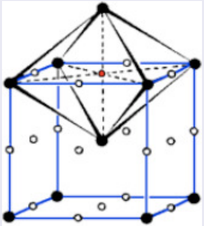
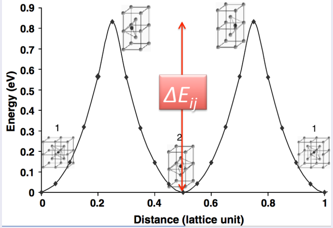
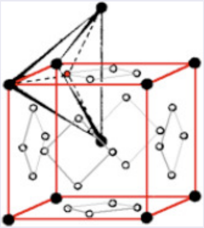
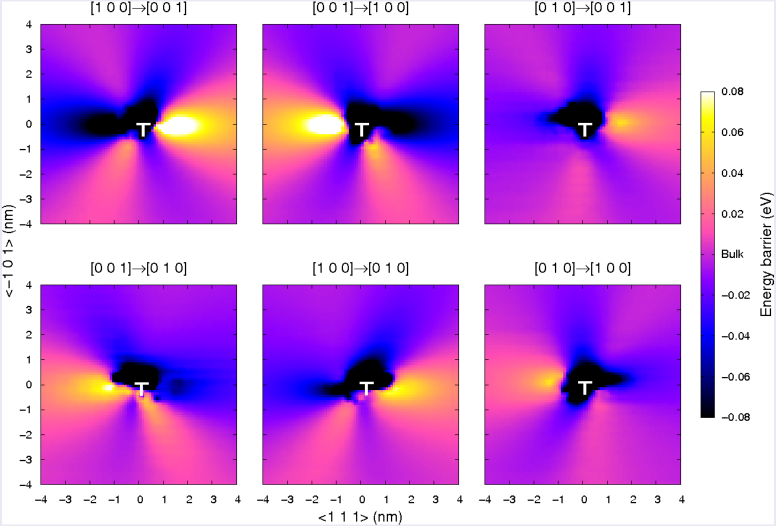






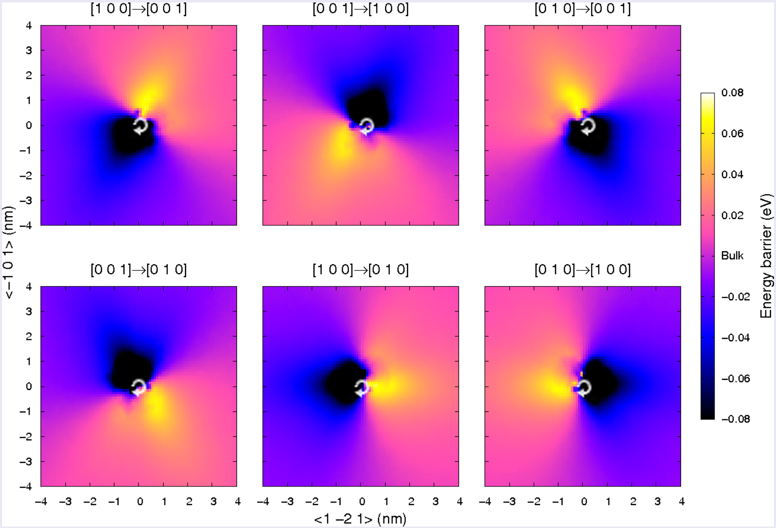
Migration energies

Edge dislocation



Migration energies

Screw dislocation



AKMC simulations

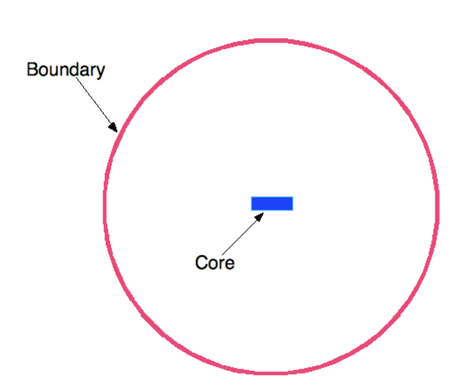
From migration energies to overall kinetics

- AKMC → rigid lattice → o-sites connected by t-sites
- Carbon diffusion investigated within a radius of 10 nm around the dislocation line
- Temperatures in the 300–600 K range
- 200,000 trajectories per temperature
  Statistics → carbon jumps ≥ 1,000
  Randomly chosen starting point

AKMC simulations

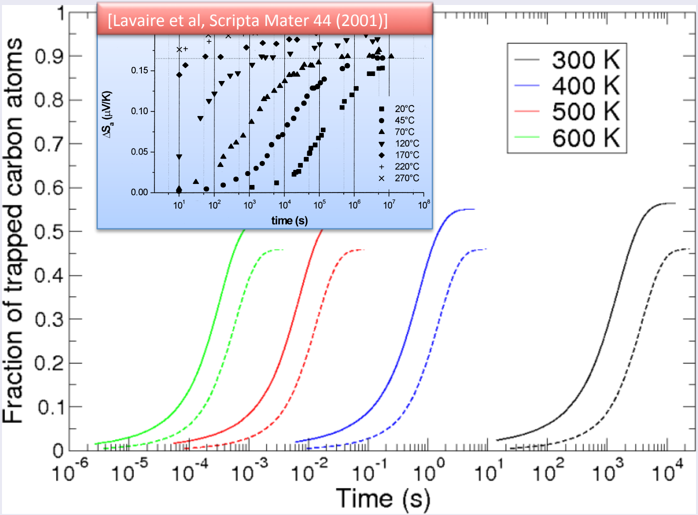
Boundary conditions

- Two end points → the “core” or the “boundary”



Results

Segregation kinetics



Bias on carbon diffusion

Mean displacement vector

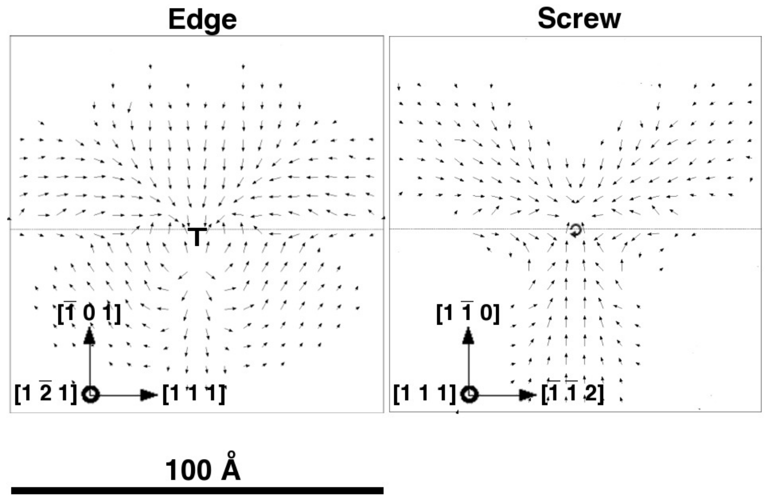
$$\overrightarrow{\epsilon} = \sum_{j=1}^{N} P_{i\to j} \overrightarrow{\delta}_{i\to j}$$

where

- $P_{i\to j} = \exp\left(\frac{-\Delta E_{i\to j}}{k_B T}\right) \to$ transition probability
- $\delta_{i\to j} \to$ jump vector from i to j
- $\vec{\epsilon} = \vec{0} \to$ simple random walk
  For all transitions :
  - Same probability
  - Same jump distance
- $\vec{\epsilon} \neq \vec{0} \to$ biased random walk

Bias on carbon diffusion

$|\vec{\epsilon}| \geq 0.01$ Å, for T=300 K



Comparison with elasticity theory

What is elasticity theory ?

- BCC $\rightarrow$ Anisotropic !
- Carbon : "elastic dipole"
- Associated force moment tensor P_{ij}
- Stress :

$$\sigma_{ij} = -\frac{1}{V} P_{ij}$$

- Dislocation : elastic deformation ϵ_{ij}^d
- Binding energy in octahedral sites AND tetrahedral sites :

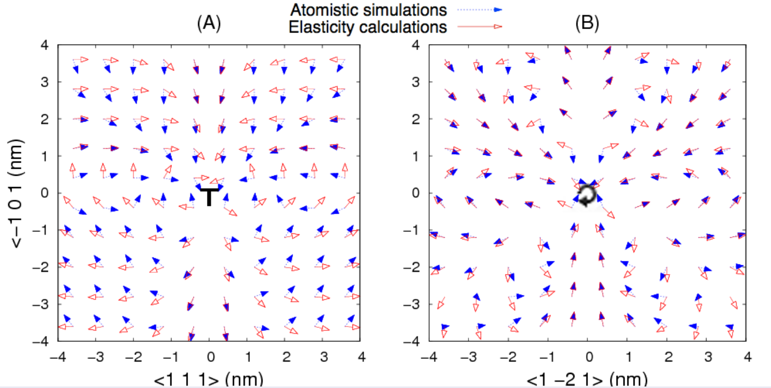
$$E_b^{o/t} = P_{ij}^{o/t} \cdot \epsilon_{ij}^d$$

- Energy barrier :

$$\Delta E = E_b^t - E_b^o$$

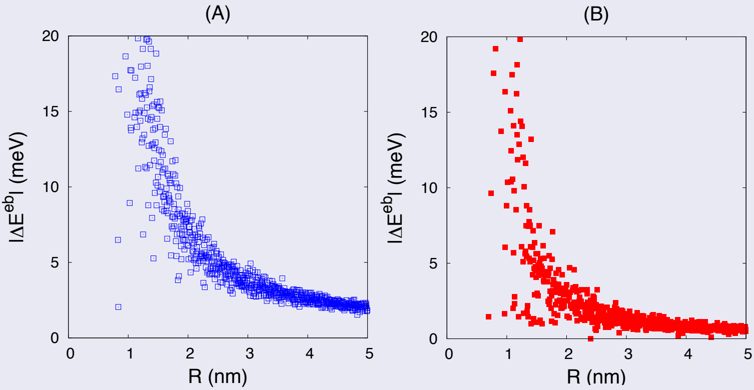
Comparison with elasticity theory

Bias on carbon diffusion



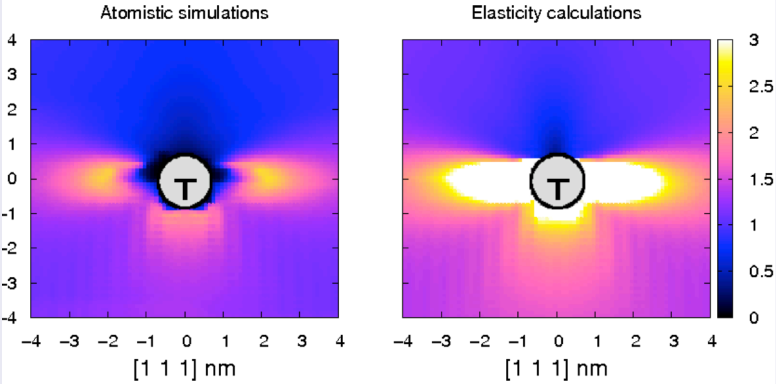
Comparison with elasticity theory

Energy barrriers



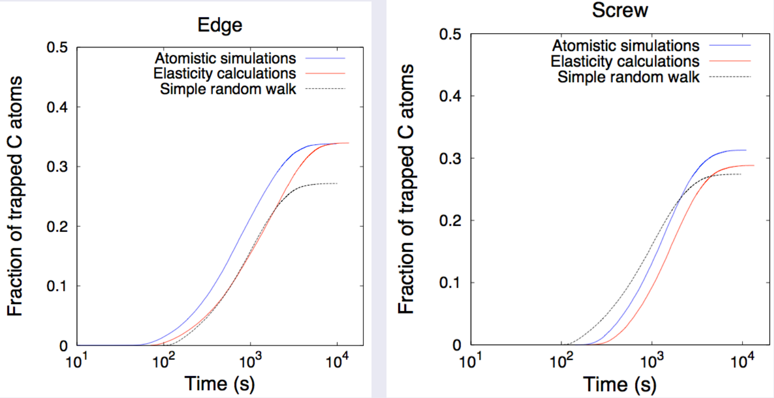
Comparison with elasticity theory

Residence time (s)



Comparison with elasticity theory

Segregation kinetics



So far...

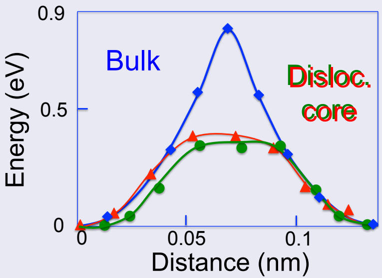
Summarizing...

- Carbon diffusion in the vicinity of a dislocation $\rightarrow$ biased random walk
- Carbon jumps faster as it gets close to the dislocation line
  - This effect decreases quickly with increasing temperature
- Attractive effect (compared to the bulk case)
- Edge effect more important than screw

Work in progress

MS+AKMC : carbon diffusion in the dislocation core

- Mapping energy minima in the core of dislocations (MS)
- Energy barriers → Nudged elastic band (MS)
- Carbon diffusion in the pipe (AKMC)



Towards AℓEMI : a few ideas

MS+AKMC : solute migration to α/γ interface

- Fe-C-X potential from Fe-C and Fe-X ?
- diffusion across the interface ?

MS : towards a better understanding of X_X^*

- effect of the interface "roughness" ?

MD+MC/KMC :interface migration

- Interface migration with MC
- Solute diffusion with KMC

Thanks for your attention !