Modelling static and dynamic strain ageing in FeC alloys

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Project Capes-Cofecub: PH 770 13
Objectives:

Understand the formation of Cottrell atmospheres, and the strain effect associated in FeC and FeMnC model steels.

Strain ageing effects in metallic alloys observed at the macroscopic scale but originate from physical phenomena arising at an atomic scale.

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**Figure 1.1**: Typical traction curve with Luders bands.

**Figure 1.2**: Typical traction curve with Portevin-Le Chatelier heterogeneities.

PhD Belotteau, Centrale Paris, 2009

Cottrell atmosphere of boron atoms in the core of an edge dislocation in aluminium

D. Blavette et al / Science, 286 (1999) 2317
Understand the formation of Cottrell atmospheres, and the strain effect associated in FeC and FeMnC model steels.
Cottrell and Bilby theory:

- Dislocations introduced by plastic deformation interact with interstitial C atoms in solid solution through their respective stress fields.

  ==> carbon segregation to dislocations

- More C atoms segregate: an “atmosphere” grows around the dislocations.

- Cottrell atmosphere hinders the dislocation motion upon reloading, such that a higher stress is required in order to make the dislocation tear away from the solutes.

Cottrell atmosphere formation = first stage of static strain aging. Second stage = carbide precipitation in the dislocation vicinity.

Hardening / softening behaviour of C atoms

Fig. 1. Experimental activation area $\mathcal{A}$ and yield stress $\tau$ as functions of temperature $T$ in Fe and FeC. The yield stress is taken as the resolved shear stress on the most stressed plane, and in a $\langle 111 \rangle$ direction (strain rate $1.7 \times 10^{-4}$ s$^{-1}$). From Kuramoto et al. [6].

D. Caillard, Acta Mater. 59 (2011) 4974
PhD Quoc Hoang Nguyen: atomic simulation of C- screw dislocation in Fe: impact on plasticity december 2009

- One screw dislocation
- One C atom

FeC potential: predicts correctly screw disl. core configuration and $E_{\text{mig}} \text{C}$ [Becquart]

soft (or easy) core: **stable**.
hard core: **métastable**.

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Binding energy between C and a screw dislocation

Elasticity theory
$E_b = 0.5 \text{ eV} \ [\text{Kamber}]$
$E_b = 0.70 \text{ eV} \ [\text{Cochard}]$

Experiments
$E_b = 0.45 \text{ eV} \ [\text{Henderson}]$
$E_b = 0.75 \text{ eV} \ [\text{Gavril'yuk}]$

Binding energy between C and a screw dislocation: Comparison with anisotropic elasticity theory

$E_{\text{binding}}^{\text{screw-octa}} = \sigma_{ij}^{\text{screw}} \cdot \varepsilon_{ij}^{\text{octa}} \cdot \Omega_{\text{box}}$

$0.1 \text{ eV}$

$0.2 \text{ eV}$

$r > 1.5 \text{ Å}$

Disagreement with anisotropic elasticity theory

Curvature of the line in the vicinity of C atom $\rightarrow$ local effect

confirmed recently by DFT [Ventelon]

Motion of dislocation facing a C atom

One screw dislocation and one C atom

3 behaviors:

- **C immobile, slip on \{110\}**
  - C115

- **C immobile, cross slip \{112\}**
  - C131

- **C changes site, slip on \{110\}**
  - C132

- Critical shear stress decreases when T increases

- Dislocation pinning at low T (100K) → not observed at higher T (300 & 500 K)
Roberto Veiga PhD thesis: September 2011: Computational insights into the strain aging phenomenon in bcc Fe at the atomic scale

1/ Carbon diffusion in the vicinity of dislocations

2/ Carbon diffusion in the core of a dislocation

3/ Carbon distribution in a Cottrell atmosphere
1/ Carbon diffusion in the vicinity of a dislocation

200,000 KMC simulations = paths followed by 200,000 non-interacting carbon atoms.

Edge dislocation:
- C trapping ($\approx 34\%$ vs. $27\%$)

Screw dislocation:
- C trapping ($\approx 32\%$ vs. $27\%$)

1/ Carbon diffusion in the vicinity of a dislocation

Figure 3. Strain ageing kinetics of ULC steel after cold rolling (50% of reduction) for different temperatures.

TEP measurements obtained from Lavaire et al.

Number of carbons arriving at an edge dislocation calculated by KMC.

TEP: Sensitive to carbon content in solid solution, but not in the dislocation, KMC results can be compared to TEP (in principle)
2/ Carbon diffusion in the core of a dislocation

Within $R < 1$ nm: distorted lattice --> T-site as saddle point assumption no longer valid --> $E_m$ calculated with the NEB

Large variation of $E_m$ near the dislocation line

Lowest $E_m$:
0.14 eV (edge)
0.19 eV (screw)

Highest $E_m$:
1.55 eV (edge)
1.14 eV (screw)
2/ Carbon diffusion in the core of a dislocation

From long trajectories (1,000,000 jumps) at high $T$:
- Calculate $D = \langle [z(t)]^2 \rangle / 2t$
- Activation energy --> slope $\log D(1/T)$
  - 0.67 eV (edge)
  - 0.74 eV (screw)
  - 0.82 eV in the bulk

Agreement with exp: enhanced diffusivity in the dislocation channel [Legros]

3/ Carbon distribution in a Cottrell atmosphere

Statistical model (Louat) based on the binding energies + MC

3/ Carbon distribution in a Cottrell atmosphere

Statistical model (Louat) based on the binding energies + MC


<table>
<thead>
<tr>
<th>Method</th>
<th>References</th>
<th>Dislocation</th>
<th>Extent (nm)</th>
<th>$\epsilon_{fac}$</th>
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<td>Molecular statics</td>
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<td>Edge</td>
<td>15 x 6</td>
<td>6.3</td>
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<tr>
<td></td>
<td>This work</td>
<td>Screw</td>
<td>8 x 8</td>
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<tr>
<td>Elasticity+DFT</td>
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<td>20 x 20</td>
<td>5.3</td>
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<tr>
<td></td>
<td>[Hanlumyuang 2010]</td>
<td>Screw</td>
<td>12 x 12</td>
<td>4.4</td>
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</tbody>
</table>
1/ Carbon diffusion in the vicinity of dislocations: C atoms are attracted to dislocation cores

2/ Carbon diffusion in the core of a dislocation: confirmation of pipe diffusion

3/ Carbon distribution in a Cottrell atmosphere: enrichment factor in agreement with exp.
Dislocation glide in Fe–carbon solid solution: From atomistic to continuum level description

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-C solution: resistance of \{112\} slip plane lower than that of \{110\} plane.
-Complex collective effect of C atoms coupled with the residual lattice friction
  => weak softening effect could take place

Fig. 7. Stress–strain curves for 1/2[111](112) edge dislocation overcoming a C atom at different positions, (a) Anti-twinning shear and (b) twinning shear.
Monte Carlo and molecular dynamics simulations of screw dislocation locking by Cottrell atmospheres in low carbon Fe–C alloys

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New model to build atmosphere: around a screw dislocation

Fig. 1. MC-equilibrated carbon Cottrell atmospheres at T = 300 K for the systems with (a) 20, (c) 140 and (b) 500 ppm of carbon. Only non-bcc iron atoms (small red balls) and the carbon atoms (big blue balls) are shown for clarity. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 3. (a) Stress required to unpity the screw dislocation from the Cottrell atmosphere as a function of carbon content; (b) Stress–strain curves associated with the systems containing 500 ppm of carbon. ATM is Cottrell atmosphere; SS is solid solution.

==> Very high unpinning stresses compared to C solid solution.

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Cottrell atmosphere formation at the atomic scale: k-ART. *Comparison with Metropolis MC and O. Waseda’ PhD work.*

Dislocation – Cottrell atmosphere interactions at the atomic scale: *determination of the upinning stress (MD) at various temperatures and for atmospheres containing different levels of C or Mn (using existing FeC and FeMn potential), C and Mn (if a FeMnC potential is published).*

Cottrell atmosphere re-formation at the atomic scale: k-ART
*Kinetic of C atoms rearrangement after the dislocation has moved away from the Cottrell atmosphere.*

Cottrell atmosphere and dislocation motion at the mesoscale: phase field
*Possibility to study collective dislocation interactions.*
I37 <111> loop

b = ½ <111>
I37 <111> loop: structure

Common neighbour analysis OVITO
I19 \langle 111 \rangle\) loop: structure

Common neighbour analysis OVITO

- **bcc**
- **other**

The **torus geometry is valid** for quite small loop sizes
Distances similar: the relaxation with EP not very large most of the time.

DFT and EP relax differently.
C-119 loop binding energy

- Eb empirical potential (eV)
- Eb DFT (eV)

(1458 + 19) AV
1458 AV
DFT more sensitive to box volume
C-119 loop binding energy
distance between loop center of mass and C atom

EP + box + 19 atomic volumes
C- I19 loop binding energy

DYMOKA 1477 AV

EP + box + 19 atomic volumes

Repulsion inside the loop
- The highest binding energy sites have the highest coordination number
- Good trends with the Voronoi volume
C-I19 loop binding energy

Empirical potential
C- I19 loop binding energy

DFT: 1458 AV

DFT: 1477 AV

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UMET

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K-ART

Special thanks to
Calcul Québec
Calcul Canada

-300 K
-1478 atoms: 19 SIA <111> loop + 1 C atom
-300 K lattice parameter + 19 atomic volumes

-12 processors
K-ART simulations at 300 K

- 1477_1469: -0.09 eV
- 1472_1474: -0.09 eV
- 1402_1392: 0.16 eV
- 1396_1353: 0.3 eV
- 1375_1383: 0.39 eV
- 1361_1405: 0.53 eV

CM - C distance (Å)

Time (s)
K-ART simulations at 300 K
Method 1: the C atom (red atom) is placed near the Fe (blue atoms) loop

Method 2: all the transitions with an energy $< 0.2$ eV are ignored $\Rightarrow$ only the C will move
Average time step for a C jump: $\sim 8.10^{-8}$ s  
Average time step for a loop displacement: $\sim 8.10^{-15}$ s.

The loop moves way faster than the C atom $\implies$ the loop needs to be pinned for the atmosphere to form.
Average time step for a C jump: $\sim 8 \times 10^{-8}$ s
Average

The loop needs to be pinned.

MD: 300 K.
$Dt = 3 \times 10^{-15}$ s
Total time: 1.5 ns
Box = 11 x 11 x 11 u.c.
Perspectives

- On going work
- Pin the loop with many C atoms
- Couple k-ART with regular AKMC with Lincos approach