Atomistic modelling of phase transformation at large time and length scales: atomistic phase field approach

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Acknowledgements

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Microstructure of alloys

Order-disorder phase transition

Phase separation

L12 ordered particles

Ni-8%Al-6%Ti aged at 800°C during 45h

J Boisse et al Acta Mat. 55, 2007
Displacive transformations

R. Hossain et al Mat. Charact. 149, 2019

Microstructures of the steel


cubic $\rightarrow$ trigonal martensitic transformation in a polycrystalline system
An APT analysis of HPT 400 °C 316 steel reveals formation of Mo–Cr–Si rich segregation at a grain boundary—Mo and Si atoms are displayed.

Landau-Khalatnikov kinetic equation (1954)

\[ \frac{d\psi(\vec{r}, t)}{dt} = -\gamma \frac{\partial F}{\partial \psi(\vec{r}, t)} \]

Landau-Khalatnikov relaxation equation

Atomistic description (nm)

Microscopic kinetic equation

Atomic density function theory

\[ \frac{dP(\vec{r}', t)}{dt} = \sum_{\vec{r}'} L(\vec{r} - \vec{r}') \frac{\partial F}{\partial P(\vec{r}', t)} \]

Continuos field description (\(\mu\)m)

Time dependent Ginzburg-Landau equation

\[ \frac{\partial \eta(\vec{r}, t)}{\partial t} = -L \left( \frac{\delta F}{\delta \eta(\vec{r}, t)} \right) + \zeta_\eta(\vec{r}, t) \]

Cahn-Hilliard equation for concentrations

\[ \frac{\partial c(\vec{r}, t)}{\partial t} = \nabla M \nabla \left( \frac{\delta F}{\delta c(\vec{r}, t)} \right) + \zeta_c(\vec{r}, t) \]

Phase field variables:

- Concentration \(c(\vec{r})\)
- Orde parametre \(\eta(\vec{r})\)

\(P(\vec{r})\) is the probability to find atom in position \(\vec{r}\).

\(\eta=1\)

\(\eta=0\)
Addressable Scales

Spatial scales:
- Atomic scale
- Nano-scale
- Micron and sub-micron scale

Time scale: sub-second - up to years

Phenomenological approaches

Discret description

Continuous approach

Atomic density function

Quasiparticle Approach
Phase Field Crystal
From Phase Field to Phase field Crystal Model

**Stability of the system with respect to infinitesimal fluctuations**

\[ \delta c(r) = c(r) - \bar{c} \]

Free energy of heterogeneous system in continuous approximation

\[
F = \int_{\mathcal{V}} \left[ (f(c) + \frac{1}{2} \beta(c)(\nabla c)^2) \right] dV
\]

Variation of free energy with respect to small fluctuations

\[ \delta c(r) = c(r) - \bar{c} = \frac{1}{N} \sum_k c(k)e^{ikr} \]

\[
\Delta F = \frac{1}{2} \int b(k) \left| c(k) \right|^2 \frac{d^3k}{(2\pi)^3}
\]

\[
\min F \quad \rightarrow \quad \min b(k)
\]
Two types of minima:

- \( k=0 \) separation
- \( k \neq 0 \) periodic structures

\[
\frac{\partial b(k)}{\partial k} \bigg|_{k=k_j} = 0
\]
Brazovskii model of crystalisation

The addition $\Psi^3$ in the free energy functional break $\pm$ symmetry (Brazovskii energy, 1975)

\[
F = \int d\mathbf{r} \left[ \frac{1}{2} \psi(-\varepsilon + (k_0^2 + \nabla^2)^2)\psi + \alpha \frac{\psi^3}{3} + \frac{\psi^4}{4} \right]
\]

for $\varepsilon=3/4$ and $k_0=1$
\[ \frac{\partial \psi}{\partial t} = -L \frac{\delta F}{\delta \psi} = L(\varepsilon - (q_0^2 + \nabla^2)^2 \psi - \alpha \psi^2 - \psi^3) \]

Swift-Hohenberg model of convection

stripes

honeycomb structure.

Rayleigh–Bénard convection

Phase Field Crystal method (K. Elder, 2002) -> zones with high concentration -> atoms
Limit transition to the Landau theory

\[
F = \int \frac{1}{2} \sum_{\alpha \beta} V_{\alpha \beta}(k) \Phi_{\alpha}(k) \Phi^{*}_{\beta}(k) \frac{d^3k}{(2\pi)^3} + \int_{V} f(\{\rho_{\alpha}(r)\})d^3r
\]  

(1)

Where \( V_{\alpha \beta}(k) \) is the Fourier transforms of the effective potentials \( W_{\alpha \beta}(r) \):

\[
V(k) = \int_{V} W(r) \exp(-ikr) d^3r
\]

Using Taylor expansion of \( V_{\alpha \beta}(k) \) in \( k \)

\[
V_{\alpha \beta}(k) = A_0^{\alpha \beta} + \frac{1}{2!} A_2^{\alpha \beta} k^2 + \frac{1}{4!} A_4^{\alpha \beta} k^4 + ... + \frac{1}{n!} A_n^{\alpha \beta}
\]

Eq.(1) is a generalized Landau gradient expression:

\[
F = \int_{V} \sum_{\alpha \beta} \left( \frac{1}{2!} A_0^{\alpha \beta} \rho_{\alpha}(r) \rho_{\beta}(r) + \frac{1}{2!} A_2^{\alpha \beta} \nabla \rho_{\alpha}(r) \nabla \rho_{\beta}(r) + \frac{1}{4!} A_4^{\alpha \beta} \nabla^{2} \rho_{\alpha}(r) \nabla^{2} \rho_{\beta}(r) + ... \right) d^3r
\]

\[
+ \int_{V} f(\{\rho(r)\}) d^3r
\]

The Phase Field Crystal model has used two first terms of the gradient expansion of the Landau theory.
From Atomic density function theory on constrained lattice to continuous approach

\[ F = F_{\text{chem}} + E_{\text{elast}} \]

\[ F_{\text{chem}} = \frac{1}{2} \sum r,r' V(r-r')p(r)p(r') + k_B T \sum \{ p(r) \ln(p(r)) + [1-p(r)] \ln[1-(p(r))] \} \]

\[ E_{\text{elast}} = \frac{1}{2} \sum_{pq} \int \frac{d^3k}{(2\pi)^3} B_{pq}(n) \theta_p(k) \theta_q^*(k) \]

Microscopic kinetic Onsager equation

\[ \frac{dP(r,t)}{dt} = \frac{1}{k_B T} \sum_{\alpha,\beta} \sum_{r'} L_{\alpha\beta}(r-r') c_\alpha c_\beta \frac{\partial F}{\partial P(r',t)} \]

Carbide formation in Fe-C system

F. Scwab et al. submitted to Acta Mat.
Interaction potential consists of elastic and chemical parts:

\[
\tilde{W}_{pq}(\mathbf{k}) = \tilde{W}_{pq}^{\text{elas}}(\mathbf{k}) + \tilde{W}_{pq}^{\text{chem}}(\mathbf{k})
\]

\[p, q = 1, 2, 3\]
Elastic part of the interaction potential:

\[\tilde{W}^{\text{elast}}_{pq}(\mathbf{k}) = -F_{i}^{\text{oct}}(\mathbf{p}, \mathbf{k})G_{ij}(\mathbf{k})F_{i}^{\ast\text{oct}}(\mathbf{q}, \mathbf{k})\]

**Kanzaki forces**

- \[F_{x}^{\text{oct}}(3, \mathbf{k}) = -ia_{0}^{2}\sigma_{11}^{0}\sin\left(\frac{k_{x}a_{0}}{2}\right)\cos\left(\frac{k_{z}a_{0}}{2}\right)\]
- \[F_{y}^{\text{oct}}(3, \mathbf{k}) = -ia_{0}^{2}\sigma_{11}^{0}\cos\left(\frac{k_{x}a_{0}}{2}\right)\sin\left(\frac{k_{z}a_{0}}{2}\right)\]
- \[F_{z}^{\text{oct}}(3, \mathbf{k}) = -ia_{0}^{2}\sigma_{33}^{0}\sin\left(\frac{k_{z}a_{0}}{2}\right)\]

\[\sigma_{11}^{0} = (C_{11} + C_{12})u_{11} + C_{12}u_{33}\]
\[\sigma_{33}^{0} = C_{11}u_{33} + 2C_{12}u_{11}\]

**Green function**

\[G_{ij}(\mathbf{k}) = [D_{ij}(\mathbf{k})]^{-1}\]
CHEMICAL PART OF INTERACTION POTENTIAL

\[ \tilde{w}_{11}^{\text{chem}}(\mathbf{k}) = 8W_3 \cos \left( \frac{k_x a_0}{2} \right) \cos \left( \frac{k_y a_0}{2} \right) \cos \left( \frac{k_z a_0}{2} \right) + 2W_4 \left( \cos (k_y a_0) + \cos (k_z a_0) \right) + 2W_4^* \cos (k_x a_0) \]

\[ \tilde{w}_{12}^{\text{chem}}(\mathbf{k}) = 2W_1 \cos \left( \frac{k_z a_0}{2} \right) + 4W_2 \cos \left( \frac{k_y a_0}{2} \right) \cos \left( \frac{k_x a_0}{2} \right) \]

\[ W_1^{\text{chem}} = 3.13 \]
\[ W_2^{\text{chem}} = 0.87 \]
\[ W_3^{\text{chem}} = 0.27 \]
\[ W_4^{\text{chem}} = 1.4 \]
\[ W_4^{\text{chem}*} = 0.23 \]

Interaction potential

\[
\tilde{w}_{pq}(k) = -\frac{F_{i}^{\text{oct}}(p, k)G_{ij}(k)F_{i}^{*\text{oct}}(q, k)}{a_0^3 C_{44} u_{33}^2} + W_0 \frac{\tilde{w}_{pq}^\text{chem}(k)}{a_0^3 C_{44} u_{33}^2}
\]

**Dimensionless parameter**

\[a_0^3 C_{44} u_{33}^2 = 12.17 \text{ eV}\]

**Concentration expansion coefficients [1]**

\[u_{11} = -0.09\]
\[u_{33} = 0.86\]
\[t_1 = u_{11}/u_{33} = -0.1\]

**Fe\(\alpha\)**

\[a_0 = 2.865 \text{ Å}\]
\[C_{11} = 242 \text{ GPa}\]
\[C_{12} = 146.5 \text{ GPa}\]
\[C_{44} = 112 \text{ GPa}\]
Carbon diffusion in martensite phase at room temperature

$T = 40^\circ C$

$p_c = 0.4 \text{w\%}$

$t = 0$

$t = 280000$

$t = 600000$

$t = 8000000$

Figure 5.12: Dependence of the concentration $c_{\text{ch}}(r,t)$ on time at the point $r(x,y,z)$ with coordinates $(52,31,61)$. The final stoichiometric formula for the blue curve is $\text{Fe}_4\text{C}$ with an intermediate $\text{Fe}_2\text{C}$ concentration. The time units are in $t$. 
Diffraction of carbon reach zones observed after aging at room temperature

diffraction pattern obtained from Fe-15Ni-1C martensite after aging at room temperature for 26 min (K.A. Taylor et al., Met.Trans.A V.20A, 1989)

\[ \theta_{\text{obtained}} \approx 23.4^\circ \rightarrow [2 \bar{1} 0] \]

\[ \theta_{\exp} \approx 24^\circ \]

Transition-iron-carbide precipitates in a lath of tempered martensite. (a) Bright-field and (b) centered-dark-field TEM images.


\[ \eta-Fe_2C \text{ carbide} \]
From discrete to continuum ADF model

Rigide Ising lattice

\[ P(r_i, t) \]

(a) Probability \( P(r_i, t) \) to find atom on site \( r_i \)

- \( P(r) \): probability to find atom at position \( r \)
- 1 atom \( \Leftrightarrow \) 1 site

\[ \sum_r P(r) = N_{\text{atoms}} \]

Continuous model

\[ \Delta x \]

Meaning of \( P(r) \)?

\[ \sum_r P(r) \neq N_{\text{atoms}} \]

(M. Lavrskiy et al., npj computational materials 2017)

\[ \sum_r P(r) = N_{\text{fraton}} \]
The Fourier Transform representation of the model Hamiltonian:

\[
H = \frac{1}{2N} \sum_k \sum_{\alpha=1}^{\beta=m} \sum_{\beta=1}^{\beta=m} \tilde{w}_{\alpha\beta}(k) \tilde{\rho}_\alpha(k) \tilde{\rho}_\beta(k)^* 
\]

Model Potential

\[
W_{\alpha\beta}(r - r') = \theta_\alpha(r - r') \delta_{\alpha\beta} + \lambda_{\alpha\beta} W^{LR}_{\alpha\beta}(r - r').
\]

\[
\theta_\alpha(r) = \begin{cases} 
-1 & \text{if } r \leq R_\alpha \\
\xi & \text{if } R_\alpha < r \leq R_\alpha + \Delta R_\alpha \\
0 & \text{otherwise.}
\end{cases}
\]

Exemple bcc structure

\[
\hat{W}^{LR}(k) = -\exp\left(-\frac{(k - k_{b\text{cc}})^2}{2(\sigma_{b\text{cc}})^2}\right)
\]
Principal loading conditions – calculation of elastic constants

1) hydrostatic, \((x, y, z) \rightarrow (1 - \varepsilon)x, (1 - \varepsilon)y, (1 - \varepsilon)z\),
2) orthorhombic, \((x, y, z) \rightarrow (1 + \varepsilon)x, (1 - \varepsilon)y, z\)

3) monoclinique \((x, y, z) \rightarrow x + \varepsilon y, y, z\)

\[
F_{\text{cubic.}}(\varepsilon) = F_0 + V_0 \frac{3}{2} \left( C_{11} + 2C_{12} \right) \varepsilon^2
\]

\[
F_{\text{orthor.}}(\varepsilon) = F_0 + V_0 \left( C_{11} - C_{12} \right) \varepsilon^2
\]

\[
F_{\text{monoc.}}(\varepsilon) = F_0 + V \frac{C_{44}}{2} \varepsilon^2
\]
Free energy functional is:

\[
F_{\text{chem}} = \frac{1}{2} \sum_{\alpha, \beta} \sum_{r, r'} V_{\alpha \beta} (r - r') p_\alpha (r) p_\beta (r') + k_B T \sum_{\alpha} \sum_{\tilde{r}} \left[ p_\alpha (r) \ln [p_\alpha (r)] + [1 - p_\alpha (r)] \ln [1 - (p_\alpha (r))] \right]
\]

Reduced variables:
- **time** is measured in units of typical atomic migration time, \( \tau_0 \)
- **energy** is measured in units of \( k_B T_0 \), where \( T_0 \) is the solidification temperature
- **the grid lattice increment**, \( l \), (the spacing of the underlying Ising lattice), is defined as a fraction of the atomic radius

The numerical solution -> the semi-implicit Fourier spectral method
Self-assembly of fratons with only short range interaction

\[ \hat{\rho} = 0.1, \hat{I} = 0.5, \Delta \hat{r} = 0.17, \text{ and } \hat{T} = 0.63 \]

\[ \hat{\lambda}_1 = 45.23, \xi = 4 \]
\[ V^{sr}(r) = \begin{cases} 
-1 & \text{if } r < R \\
\xi & \text{if } R \leq r \leq R + \Delta R \\
0 & \text{if } r > R + \Delta R 
\end{cases} \]

- Short range potential:

- Long range potential\(^1\):

\[ V^{lr}(k) = 1 - \frac{k^4}{(k^2 - k_1^2)^2 + k_2^4} \]

---


GB growth (tilt angle $\theta = 3.58^\circ$)

Dislocations at GB
The atomic density function (ADF) model of tilt grain boundaries in α-Fe

Atomic configurations

GB energy

Size-Dependent Solute Segregation at Symmetric Tilt \(<100>\) Grain Boundaries in \(\alpha\)-Fe

Three types of solute atoms \(X_1\), \(X_2\) and \(X_3\) with atomic radii \(R_1 < R_{Fe}\), \(R_2 = R_{Fe}\) and \(R_3 > R_{Fe}\) corresponding to phosphorus (P), antimony (Sb) and tin (Sn).

Low angle GBs, with \(\theta = 7.15^\circ\) and \(\theta = 9.53^\circ\), and two high angle GBs, \(\Sigma 5\) (310) \((\theta = 36.95^\circ)\) and \(\Sigma 29\) (730) \((\theta = 46.40^\circ)\).

Interaction potentials

Formation of Cottrell atmospheres at $\langle 100 \rangle$ edge dislocations (red $\perp$ marks) after segregation of solute atoms at $\langle 100 \rangle$ symmetric tilt LAGBs. (a,b) $X_1$ (small) atoms segregation for a misorientation angle $\theta = 7.15^\circ$. (c,d) $X_2$ (larger) atoms for $\theta = 9.53^\circ$. (a,c) solute atoms distribution (orange) and Fe atoms (transparent). (b,d) Volume per atom variation $\Delta V / V$ (Voronoï analysis). Red—dilatation, blue—compression. $X$ atoms are spotted by green dots in (b,d).
HAGB in $\alpha$-Fe

- Solute atoms are located inside of the capped trigonal prism in dilatation region.
- With increasing of atomic size the solute atoms are concentrated more and more near GB, in dilatation region.

Figure 8. Influence of the volume per atom (Voronoi analysis) on tilt $\Sigma$ of $X_1$ (a) $X_2$ (b) and $X_3$ (c) solute atoms at $\Sigma 5$ (310) ($\theta = 36.87^\circ$). $X_1$ atoms are spotted by green dots. The depleted (over-compressed) and segregated (less compressed) areas are delineated by dashed black lines, and referred to as zones 1 and 2 in (b,c).
Polycrystal in $\alpha$-Fe

$V = 70^3 \text{ nm}^3$
GRAIN BOUNDARIES STRUCTURE IN $\alpha$-IRON UNDER APPLIED STRESS: $\varepsilon=0.1$

**Equilibrium**

$\Sigma 5(310)$, $\theta = 36.87$

$\Sigma 29(730)$, $\theta = 46.40$

Under constrain
The Bain model of the martensitic transformation

**Bain OR:** \(\{010\}_\gamma \| \{001\}_\alpha\)
\(\{110\}_\gamma \| \{100\}_\alpha\)

**KS OR:** \(\{111\}_\gamma \| \{110\}_\alpha\)
\(\{101\}_\gamma \| \{111\}_\alpha\)

**Fig. 1.** Six crystallographic variants (V1–V6) for the K–S orientation relationship that evolves on a (111) austenite plane. The triangle and rectangles indicate the (111) plane of austenite (\(\gamma\): fcc) and the (011) plane of martensite (\(\alpha'\): bcc), respectively.
### MARTENSITIC TRANSFORMATIONS

The 24 crystallographic variants for the K–S orientation relationship

<table>
<thead>
<tr>
<th>Variant</th>
<th>Plane parallel</th>
<th>Direction parallel</th>
</tr>
</thead>
<tbody>
<tr>
<td>V1</td>
<td>$(111)<em>\gamma//(011)</em>{\alpha'}$</td>
<td>$[\bar{1}01]<em>\gamma//[\bar{1}1\bar{1}]</em>{\alpha'}$</td>
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<tr>
<td>V2</td>
<td>$[101]<em>\gamma//[\bar{1}1\bar{1}]</em>{\alpha'}$</td>
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<tr>
<td>V3</td>
<td>$[011]<em>\gamma//[\bar{1}1\bar{1}]</em>{\alpha'}$</td>
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<tr>
<td>V4</td>
<td>$[011]<em>\gamma//[\bar{1}1\bar{1}]</em>{\alpha'}$</td>
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<tr>
<td>V5</td>
<td>$[\bar{1}10]<em>\gamma//[\bar{1}1\bar{1}]</em>{\alpha'}$</td>
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<tr>
<td>V6</td>
<td>$[\bar{1}10]<em>\gamma//[\bar{1}1\bar{1}]</em>{\alpha'}$</td>
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<tr>
<td>V7</td>
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<td>V18</td>
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<tr>
<td>V19</td>
<td>$(11\bar{1})<em>\gamma//(011)</em>{\alpha'}$</td>
<td>$[\bar{1}10]<em>\gamma//[\bar{1}1\bar{1}]</em>{\alpha'}$</td>
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<tr>
<td>V24</td>
<td>$[101]<em>\gamma//[\bar{1}1\bar{1}]</em>{\alpha'}$</td>
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FCC-BCC transition

\[ \frac{a_0^{fcc}}{a_0^{bcc}} = \sqrt{\frac{3}{2}} \approx 1.225 \]
\[ a_0^{fcc} = 8\Delta x \]
\[ \sigma = 0.05 \]

Elastic constants of the given potential

\[ \frac{C_{11}^{bcc}}{C_{11}^{fcc}} \approx 1.68, \quad \frac{C_{12}^{bcc}}{C_{12}^{fcc}} \approx 1.25, \quad \frac{C_{44}^{bcc}}{C_{44}^{fcc}} \approx 1.3 \]

Experimental elastic constants for iron

\[ \frac{C_{11}^{bcc}}{C_{11}^{fcc}} \approx 1.60, \quad \frac{C_{12}^{bcc}}{C_{12}^{fcc}} \approx 1.15, \quad \frac{C_{44}^{bcc}}{C_{44}^{fcc}} \approx 1.51 \]

\[ \tilde{w}_{LR}(k) = \exp \left( -\frac{(k-k_0)^2}{2\sigma^2} \right) + 0.1 \exp \left( -\frac{(k-k_0)^2}{2\sigma^2} \right) \]
Twinning structure of $\alpha$-Fe (bcc) precipitate in Cu (fcc) matrix in the Cu-2.0Fe-0.5Co wt%
Growth of $\alpha$-Fe particle in the Cu matrix

Size of the simulation box $1024^3$ 46$^3$ nm

Two-variants structure with Kurdjumov–Sachs OR

G. Demange et al. Acta mat. 226 (2022)
Twin boundaries

Reflection (R) and isosceles (I) twin boundaries structures

During the propagation of TB, the transitions (I) → (R) and (R) → (I) – is accompanied by the stacking fault in \((\bar{2}11)_{\alpha_1}\) planes, which results in the shift of the interface along the direction \(\langle \bar{2}11 \rangle_{\alpha_1}\) perpendicular to the twinning plane.

Partial twin dislocation couple (IR+RI) with step
\(h = a_2(2 \sqrt{6})\), Burgers vector \(\mathbf{b} = \frac{1}{12} < \bar{1}11 >_{\alpha_1}\)
Fcc/bcc interface

3D distribution of screw dislocation cores (yellow spheres). fcc screw dislocations \( \mathbf{b}_2 = \pm 1/2\langle 110 \rangle_\gamma \)
Propagation mechanism of fcc/bcc interface

Screw dislocations:
\[ b_1 = \pm \frac{1}{2} \langle 1\bar{1}0 \rangle \gamma \]
\[ b_2 = \pm \frac{1}{2} \langle 1\bar{1}0 \rangle \gamma \]

Partial Shockley
\[ b_p = \pm \frac{1}{6} \langle 1\bar{2}1 \rangle \gamma \]

Transformation pass: fcc → hcp → bcc.
Two steps:
- Shockley partial dislocation with Burgers vector \( b_p \) produces a SF ABCABC→ ABAB
- Homogeneous deformation \( (111)_\gamma \) fcc → \( (011)_\alpha \) bcc planes (glide of \( b_1 \) and \( b_2 \) fcc screw dislocations)
Dual-phase (DP) steels

Dual microstructure of soft ferrite and harder martensite phases.

DP1000 ~ 49% ferrite
DP800 ~ 65% ferrite
DP600 ~ 75% ferrite

Bright – ferrite; dark - martensite
Role of transformation interface

Solid-state phase transformations during steel processing

Microstructure future
- phases volume fraction
- topology and morphology of phases
- grain size distribution

Mechanical properties of the steel

moving transformation interface

- Interface interaction with the alloying elements
- Orientation relationship (ORs) between two phases
- Interface properties (coherency, thickness and shape)
- Atomic structure of the interface
- Ability to dissipate energy: interfacial friction

Experimental investigation of the transformation interface at the nanoscale and modeling
15s at 625 °C: interface #7

![Image: Micrograph showing interfaces and atomic fraction profiles.]

**tip3_2nd**

\[ X_{\text{Mn}}^{\text{max}} = 4.3 \text{ at\%} \]

\[ \Gamma_{\text{Mn}} = 6 \text{ atom/nm}^2 \]

\[ \sim 1-4^\circ/\text{KS} \]

**tip5_2nd**

\[ X_{\text{Mn}}^{\text{max}} = 4.3 \text{ at\%} \]

\[ \Gamma_{\text{Mn}} = 5.5 \text{ atom/nm}^2 \]

\[ \sim 11-15^\circ/\text{KS} \]
Austenite-to-ferrite phase transformation

- The change in the crystal structure (from fcc to bcc).
- Diffusional process: the redistribution of interstitial and substitutional elements.

**Kurdjumov-Sachs (KS):**

\[
\{111\}_\gamma \parallel \{110\}_\alpha \\
\langle 101 \rangle_\gamma \parallel \langle \overline{1}11 \rangle_\alpha
\]

**Nishiyama-Wassermann (NW):**

\[
\{111\}_\gamma \parallel \{011\}_\alpha \\
\langle 10\overline{1} \rangle_\gamma \parallel \langle 100 \rangle_\alpha
\]

At higher T: disordered interfaces migrate faster
At lower T: coherent interfaces migrate faster \(^1\)
FCC-BCC plane interface

Greninger-Troiano OR

Kurdjumov-Sachs OR

Thesis Y. Borges Gomes Lima
Propagation of (575) interface with KS OR
Nishiyama Wasserman Orientation Relationship

(121) Habit plane

(575) Habit plane
FCC->BCC phase transformation in Fe

To identify the crystal defects

Slip Vector Analysis (SVA)
Nishiyama Wasserman Orientation Relationship

- Average step height: \( h = a_{BCC}\sqrt{3} \approx 0.50 \text{ nm} \).
- Average terrace length: \( 1.0 \text{ nm} \leq l \leq 1.5 \text{ nm} \).

*Slip Vector Analyses of NW (575)_{FCC} interface with a BCC reference. Blue vectors are detected dislocations mean line direction.*
Screw dislocations exist with Burgers vector $a_{fcc}/2[\bar{1}01]$ lying next to the steps along $[101]_{fcc}$, with the stacking fault between partials lying on the $(111)_{fcc}$ terrace.

F. Maresca et W. A. Curtin, Acta Mat., 134, 2017
Interaction of the Fcc/BCC interface with Carbon atoms

Long-range potential to model the C-C repulsion:

\[ w_{CC}^{LR}(r) = \begin{cases} 
0, & \text{if } r < (R_C + \Delta R_C) \\
 e^{-\alpha r}, & \text{if } r \geq (R_C + \Delta R_C) 
\end{cases} \]

\[ \alpha = 0.34 \quad [2] \]

Long-range potential to model the Fe-C repulsion (Screened Coulomb potential):

\[ w_{FeC}(r) = \frac{e^2}{r} \exp \left( -\frac{r^2}{r_D^2} \right) \]

\[ r_D = 0.2036 \cdot a_0 \] [3], where \( r_D \) - Debye radius

\[ w_{FeC}(k) = \lambda_2 \frac{1}{\left(1/r_D\right)^2+k^2} \]

\[
\hat{L}^0 = \begin{pmatrix}
L^0_{FeFe} & L^0_{FeC} \\
L^0_{FeC} & L^0_{CC}
\end{pmatrix}
\]

- \(L^0_{FeC} = 0\) - since C atoms are in interstitial positions, there is no Fe/C exchange

- \(L^0_{CC}/L^0_{FeFe} > 1\) – Carbon atoms are more mobile than iron atoms

\[
\hat{L}^0 = \begin{pmatrix}
0.67 & 0 \\
0 & 1.5
\end{pmatrix}
\]
Segregation of C atoms at non-KS interfaces

OVITO software: Common Neighbor Analysis (CAN)
• BCC;
• FCC;
• “other”;
• Carbon

\[ V = 256 \times 256 \times 512 \]
Segregation of C atoms at non-KS interfaces
3D reconstructions and concentration profiles of C and Mn atoms across (a) the 1st interface of tip5 (isothermal holding at 625°C during 15s),
(b) the 2nd interface of tip3 (isothermal holding at 625°C during 15s).

Thesis O. Nakonechna
Segregation of C atoms at fcc/bcc moving interface

FCC/BCC interface with C atoms

- Interface with Non-KS OR propagates faster than KS
- Concentration of C at non-KS OR interface is around 12%
- Concentration of C at KS OR interface is around 5-6 %
Versatility of Phase Field Atomic and Nanoscale Modeling

\[ \frac{\partial c(r,t)}{\partial t} = (\nabla M \nabla) \frac{\delta F}{\delta c} \]

\[ \frac{\partial \eta(r,t)}{\partial t} = -L \frac{\delta F}{\delta \eta} \]

Different types of fields:

- atomic density, \( \rho(r) \) – solidification, atomic ordering
- composition \( c(r) \), decomposition
- atomic LRO parameters, \( \eta(r) \), (atomic ordering)
- transformation strain, \( \varepsilon(r) \), (martensitic transformation)
- polarization, \( P \), (ferroelectrics)
- magnetization, \( M(r) \), (ferromagnets)
- Burgers vector, \( b \), (multi-dislocation systems)
- crack opening, \( h \) (multi-crack systems)