DETERMINATION OF GRAIN BOUNDARY MOBILITY IN THE FE-CR SYSTEM BY MOLECULAR DYNAMICS SIMULATION

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We have deal with the problem of recrystallisation of oxide dispersion strengthened Fe-Cr (ODS).
- Exceptional high recrystallisation temperatures (0.9 of melting temperature)
- Extremely coarse final grains, some orders of magnitude bigger than the initial microstructure

Many different recrystallisation simulations try to explain the behaviour of grain growth and migration
- Cellular automata, Monte Carlo, Finite Element Modelling, Vertex, ...

Grain boundary energy vs. Grain boundary Energy + Mobility

Grain boundary energy measures the extra energy of the atoms in the surface with respect to the bulk
- Type of boundary
- Chemistry of boundary

Grain boundary mobility measures how easy atoms transition from one grain to another grain
- Type of boundary
- Chemistry of boundary
- Dislocations
- Induced strain
- Point defects
- Pinning forces
- Triple junctions
Introduction

Curvature Constant
Mobility does not depend on curvature

Curved grain boundary simulated closer to flat grain boundary

Curvature Changes
Mobility depends on curvature

\[ \nu = M \left( \gamma_{gb} + \gamma''_{gb} \right) \left( \frac{\pi}{W} \right) = M^* \left( \frac{\pi}{W} \right) \]

Molecular Dynamics

- The classical approach of Finnis-Sinclair has been used to compute the movement of atoms
  - Good fitting with physical and mechanical properties of iron and chromium. BCC structure
    - Fe cell parameter is 2.8665 Å. Cohesive energy per atom of -4.28eV
    - Cr cell parameter is 2.8845 Å. Cohesive energy per atom of -4.10eV
  - It has been successful in modeling defects of surfaces, interactions between atoms and for calculating grain boundary energies.
  - The parameters for the pairs Fe-Fe and Cr-Cr has been chosen from the original work of Finnis and Sinclair [1-2] and for the Fe-Cr interactions, the Lorentz-Berthlot rule has been used.

Finnis-Sinclair Potential

\[
E = \frac{1}{2} \sum_i \sum_j V_{ij}(r_{ij}) - A \sum_i \sqrt{\rho_i}
\]

\[
V_{ij}(r) = \begin{cases} (r-c)^2(c_0 + c_1 r + c_2 r^2) & \text{si} \ (r \leq c) \\ 0 & \text{si} \ (r > c) \end{cases}
\]

\[
\rho_i = \sum_{i \neq j} \phi(r_{ij})
\]

\[
\phi(r) = \begin{cases} (r-d)^2 + \beta \frac{(r-d)^3}{d} & \text{si} \ (r \leq d) \\ 0 & \text{si} \ (r > d) \end{cases}
\]

Lorentz-Berthlot mixing rule

\[
c_{FeCr} = \frac{c_0^{Fe} + c_0^{Cr}}{2}
\]

\[
\beta_{FeCr} = \frac{\beta_0^{Fe} + \beta_0^{Cr}}{2}
\]

\[
c_{0}^{FeCr} = \sqrt{c_0^{Fe} \cdot c_0^{Cr}}
\]

\[
c_2^{FeCr} = \frac{c_2^{Fe} \cdot c_0^{Cr} + c_2^{Cr} \cdot c_0^{Fe}}{2 \sqrt{c_0^{Fe} \cdot c_0^{Cr}}}
\]

\[
d_{FeCr} = \frac{d_0^{Fe} + d_0^{Cr}}{2}
\]

\[
A_{FeCr} = \frac{A_0^{Fe} + A_0^{Cr}}{2}
\]

\[
c_1^{FeCr} = \frac{c_1^{Fe} \cdot c_0^{Cr} + c_1^{Cr} \cdot c_0^{Fe}}{2 \sqrt{c_0^{Fe} \cdot c_0^{Cr}}}
\]

\[
\rho(r) = \begin{cases} \rho(r) \text{ Fe Fe} \\ \rho(r) \text{ Fe Cr} \\ \rho(r) \text{ Cr Cr} \\ \rho(r) \text{ Fe Cr} \end{cases}
\]

\[
V(r) = \begin{cases} V(r) \text{ Fe Fe} \\ V(r) \text{ Fe Cr} \\ V(r) \text{ Cr Cr} \\ V(r) \text{ Fe Cr} \end{cases}
\]

c represents a cutoff parameter, c₁, c₂, c₃ are fitting parameters, d is a different cutoff parameter, A binding energy
Molecular Dynamics

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Cohesive energy in BCC is -4.28 eV (a=2.8665 Å)  
Cohesive energy in FCC is -4.23 eV (a=3.6938 Å)  

BCCₖ<FCCₖ independently of temperature so it is difficult to simulate with this potential phase transformation.

No allotropic phase transformation has been seen in FS potential  
Fe-20Cr has no phase transformation.
Simulating Grain Boundary Mobility

- Grain boundary energy is computed by setting up two different orientations and defining a connecting plane
  - No curvature => No curvature driven mobility measurement is possible
  - The initial configuration of the grain boundary energy computations are not able to say anything about mobility.
- We need a curved boundary to have a pressure on the surface.

\[ S_i = \sum_j \cos \left( \frac{(k \cdot r_i - k \cdot r_j)}{2\pi a} \right) \]

\[ v = M \cdot P ; \quad M = M_0 \exp(-Q/kT) ; \quad P = \frac{\gamma_{gb} + \gamma_{gb}}{R} ; \quad v = M \cdot \frac{\gamma_{gb} + \gamma_{gb}}{R} = M \frac{1}{R} \]
Grain Boundary Choice

- **<110> Symmetric Tilt Grain boundary:**
  - Mechanically alloyed metals has in general has a <110> fiber tilt boundary characteristics
  - Obviously it can be represented LAGB and HAGB
  - CSL nomenclature (coincident site lattice) has influence in some cases
    - It is of paramount importance in some specific cases, although in general LAB or HAB have higher effect on grain boundary properties.
  - In general tilt boundaries (symmetric or asymmetric) are the most common boundaries
    - Symmetrical tilt boundaries are very useful for molecular dynamic simulations. Easy boundary conditions
  - We have previous information about this family


Grain Boundary Choice

- <110> Symmetric Tilt Grain boundary:

\[ \gamma = \frac{E_{\text{tot}} - CE(T) \cdot N_{\text{atoms}}}{2 \cdot A} \]

Grain Boundary Energy in the Fe-20%Cr system with respect to Misorientation and Temperature

Evolution of Grain Boundary energy with respect to %Cr

Grain Boundary energy with respect to temperature in Pure Fe
Grain Boundary Set Up

- Segregation must be considered if two different kind of atoms are involved
  - Why? ..... Previous evidences in very pure system (Al), just a little amount of impurities can affect drastically the mobility
    - 99.9992 % Al is two orders of magnitude lower than 99.99995 %Al
  - Experimental results on mechanically alloyed metals did not detect segregation in the boundary or in the bulk
    - High recrystallization temperature
    - Kinematics of diffusion are slower than cooling process
    - Similar atoms Fe-Cr. Other “less” similar atoms can affect
    - Oxide particles
    - Predominant Low angle misorientation
    - ...

\[ E_s = -0.16 \text{ eV} \]

\[ C_d = \frac{C \cdot e^{E_s/kT}}{1 - C + C \cdot e^{E_s/kT}} \]

Simulation Results

- **Case 11.5°**
  - Low mobility
    - $M^* = 4 \times 10^{-9} \text{ m/s}^2$
  - High Activation Energy
    - $Q = 1.25 \text{ eV}$
  - Low grain boundary energy
    - $\gamma = 1 \text{ J/m}^2$

- Grain boundary structure
Simulation Results

- **Case 26.5°**
  - **High Mobility**
    - $M^* = 9 \times 10^{-9} \text{ m/s}^2$
  - **Low Activation Energy**
    - $Q = 0.61 \text{ eV}$
  - **High grain boundary energy**
    - $\gamma = 2.2 \text{ J/m}^2$

- **Grain boundary structure**
Simulation Results

- **Case 109°**
  - Very High mobility
    - \( M^* = 15 \times 10^{-9} \text{ m/s}^2 \)
  - Very Low Activation Energy
    - \( Q = 0.27 \text{ eV} \)
  - Low grain boundary energy
    - \( \gamma = 0.7 \text{ J/m}^2 \)

- Grain boundary structure
Simulation Results

- **Case 50.4°**
  - Low mobility
    - $M^* = 2.4 \times 10^{-9} \text{ m/s}^2$
  - Medium Activation Energy
    - $Q = 0.71 \text{ eV}$
  - High grain boundary energy
    - $\gamma = 1.7 \text{ J/m}^2$

- Grain boundary structure
We have computed a set of representative boundaries for three different medium and high temperatures.

A Previous work [1] reports similar mobility in ODS PM2000 (Fe-20Cr-5Al), although an activation energy significantly higher than simulations:

Conclusions

- Hat-shape geometry has been tested to compute mobility in the Fe-Cr system without segregation in the boundaries.
- LAGB has in general lower mobility than HAGB.
- But LAGB / HAGB classification is not enough to classify the mobility of a boundary.
  - Configuration of atoms affects mobility as well as affects grain boundary energy.
  - Low energy in HAGB has very high mobility.
  - Some HAGB behave as LAGB.
- It seems to be a relationship between grain boundary energy and mobility.
- Previous works [1] report similar mobility in ODS PM2000 (Fe-20Cr-5Al), although an activation energy significantly higher than simulations:
  - Pinning particles.
  - More elements.
  - Texture dominated by LAGB.
- Future work:
  - Comparison with U-shape bicrystal geometry.
  - Stress induced mobility.
  - Longer simulations with segregation at the boundaries.
  - Effect of Dislocations and vacancies.
  - More elements (Al).
  - ...


Thank you for your attention.