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

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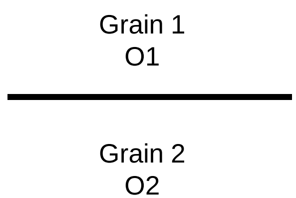
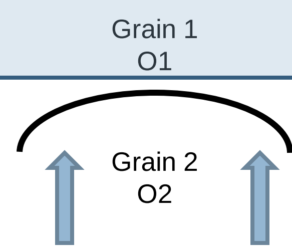
Introduction

- 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

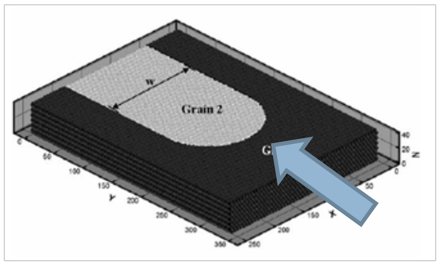




Grain boundary mobility measures how easy atoms transition from one grain to another grain

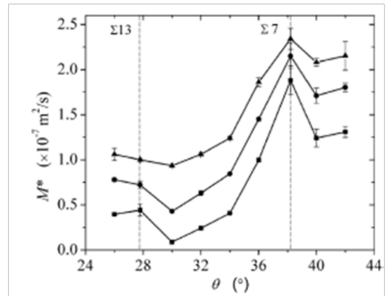
- Type of boundary
- Chemistry of boundary
- Dislocations
- Induced strain
- Point defects
- Pinning forces
- Triple junctions

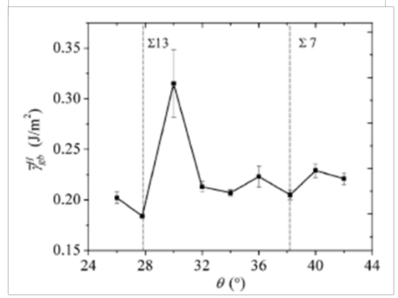
Introduction

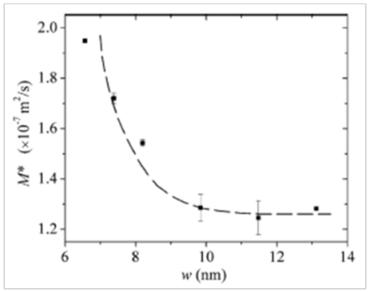


H. Zhang et al. / Acta Materialia 53 (2005) 79–86

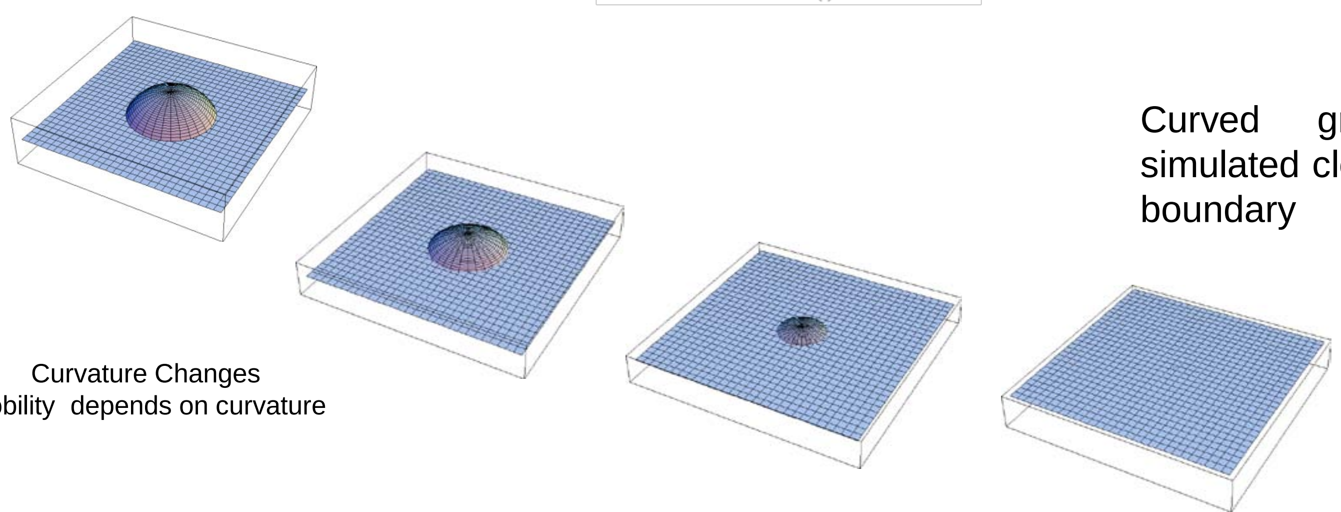
$$\upsilon = M(\gamma_{gb} + \gamma''_{gb})\left(\frac{\pi}{w}\right) = M^*\left(\frac{\pi}{w}\right)$$







Curvature Constant
Mobility does not depend on curvature



Curved grain boundary simulated closer to flat grain boundary

Curvature Changes
Mobility depends on curvature

Molecular Dynamics

- The classical approach of Finnis-Sinclair has been used to compute the 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

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

$$V_{ij}(r)=\begin{cases}(r-c)^2(c_0+c_1r+c_2r^2) & \text{si}\quad (r\le c)\\ 0 & \text{si}\quad (r>c)\end{cases}$$

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

$$\phi(r)=\begin{cases}(r-d)^2+\beta\dfrac{(r-d)^3}{d} & \text{si}\quad (r\le d)\\ 0 & \text{si}\quad (r>d)\end{cases}$$

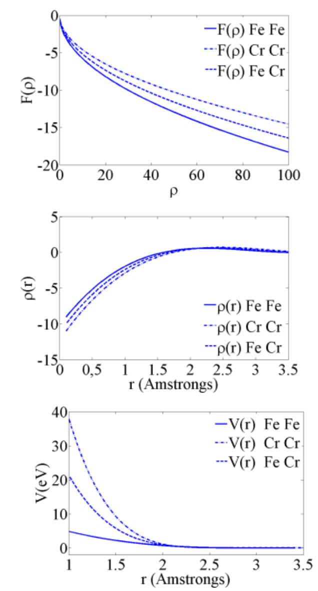
Lorentz-Berthlot mixing rule

$$c^{FeCr}=\frac{c^{Fe}+c^{Cr}}{2}\qquad d^{FeCr}=\frac{d^{Fe}+d^{Cr}}{2}$$

$$\beta^{FeCr}=\frac{\beta^{Fe}+\beta^{Cr}}{2}\qquad A^{FeCr}=\frac{A^{Fe}+A^{Cr}}{2}$$

$$c_0^{FeCr}=\sqrt{c_0^{Fe}\cdot c_0^{Cr}}\qquad c_1^{FeCr}=\frac{c_1^{Fe}\cdot c_0^{Cr}+c_1^{Cr}\cdot c_0^{Fe}}{2\sqrt{c_0^{Fe}\cdot c_0^{Cr}}}$$

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



c represents a *cutoff* parameter, c_1, c_2, c_3 are fitting parameters, *d* is a different *cutoff* parameter, *A binding energy*

Molecular Dynamics

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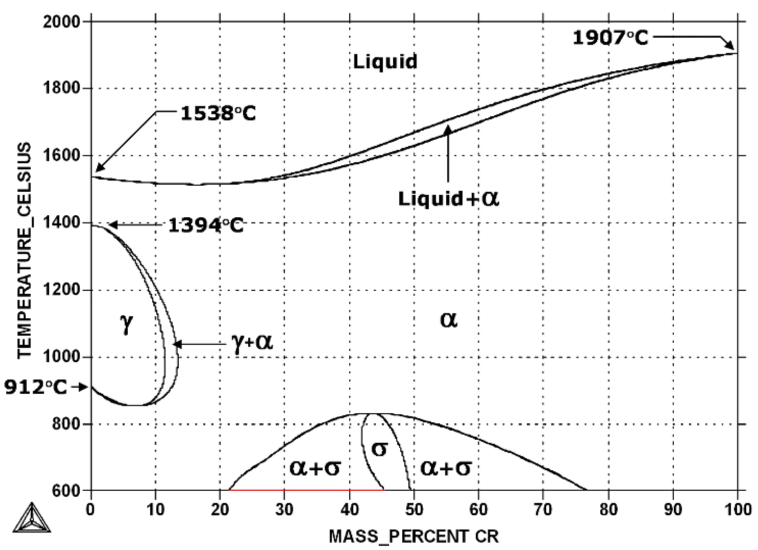


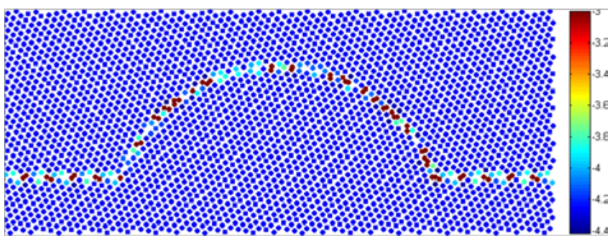
Cohesive energy in BCC is -4.28 eV (a=2.8665 Å)
Cohesive energy in FCC is -4.23 eV (a=3.6938 Å)

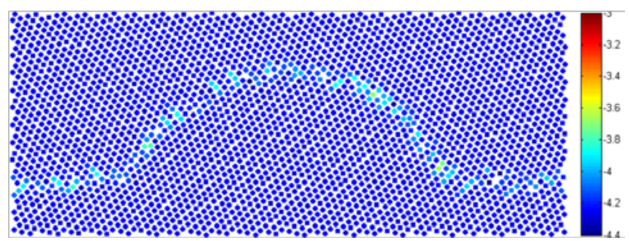
BCC_E<FCC_E independently of temperature so it is difficult to simulate with this potential phase transformation.

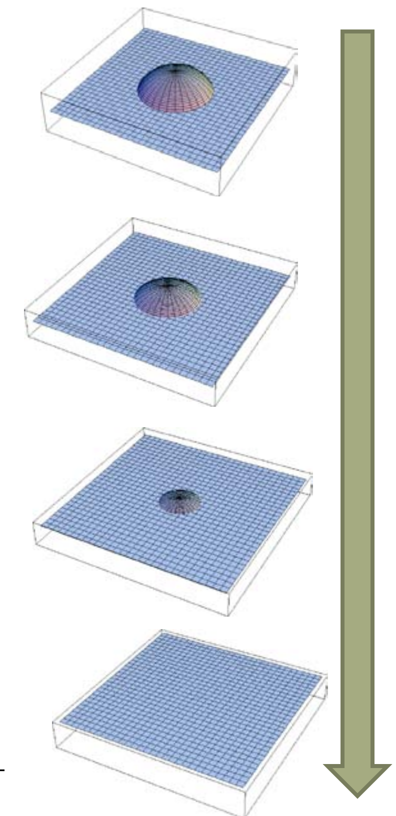
No allotropic phase transformation has been seen in FS potential Fe-20Cr has no phase transformation.

Simulating Grain Boundary Mobility

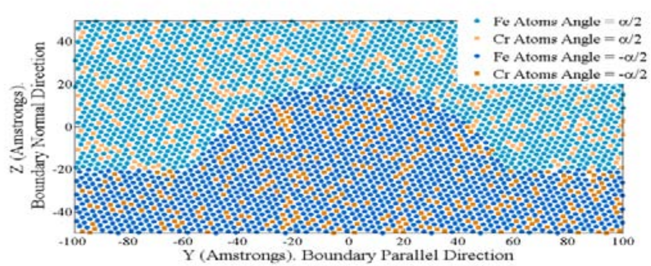
- Grain boundary energy is computed by setting up two different orientations and defining a connecting plane
  - No curvature => No curvature driven mobility measurement is possible
  - The initial configuration of the grain boundary energy computations are not able to say anything about mobility.
-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







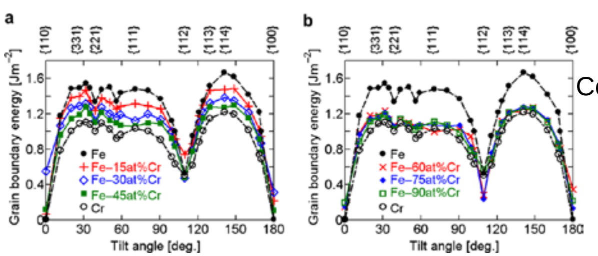
$$S_i = \frac{\sum_j \cos\left((k \cdot r_i - k \cdot r_j)/a\ 2\pi\right)}{n^2}$$



$$v = M \cdot P \quad ; \quad M = M_0 \exp(-Q/kT) \quad ; \quad P = \frac{\gamma_{gb} + \gamma_{gb}}{R} \quad ; \quad v = M \cdot \frac{\gamma_{gb} + \gamma_{gb}}{R} = M * \frac{1}{R}$$

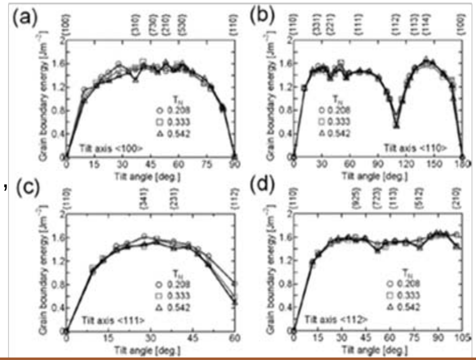
Grain Boundary Choice

- <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



Y. Shibuta, et al. Computational Materials Science 44 (2009) 1025–1029

Y. Shibuta et al. ISIJ International, Vol. 48 (2008), No. 11, pp. 1582–1591



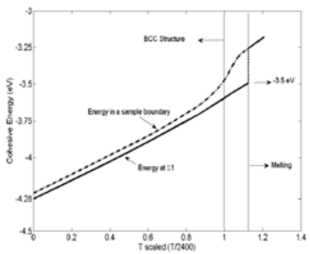
Evolution of Grain Boundary energy with respect to %Cr

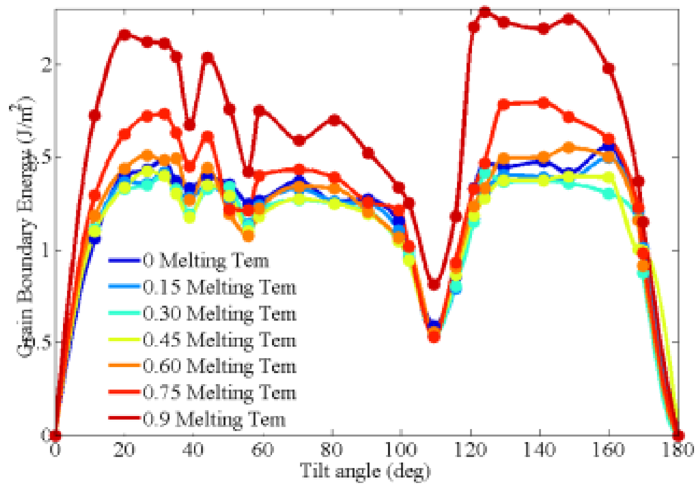
Grain Boundary energy with respect to temperature in Pure Fe

Grain Boundary Choice

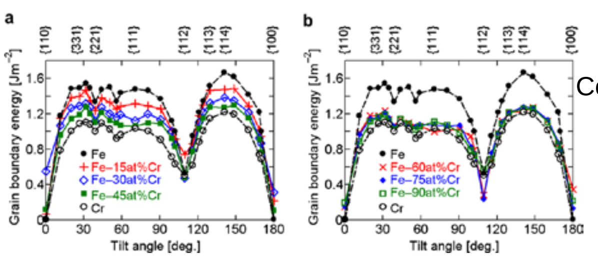
- <110> Symmetric Tilt Grain boundary:

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





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



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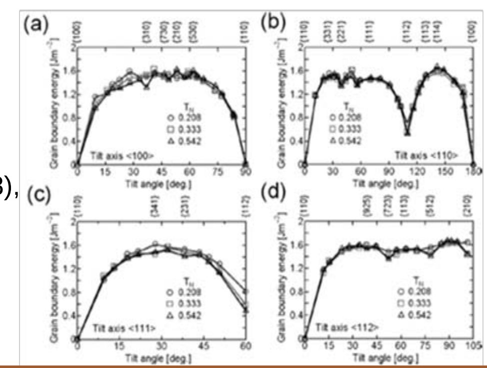


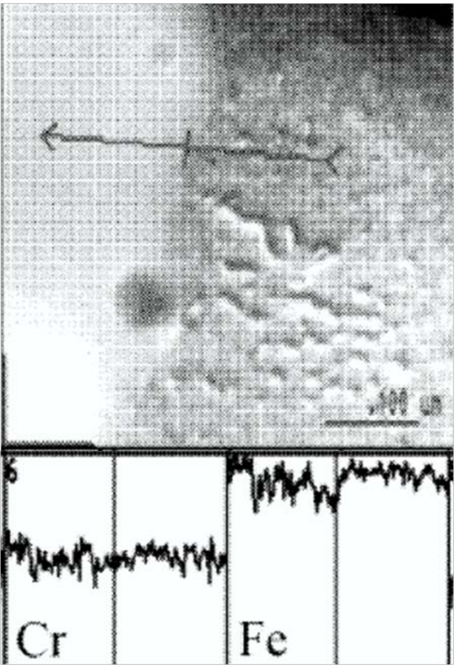
Evolution of Grain Boundary energy with respect to %Cr

Grain Boundary energy with respect to temperature in Pure Fe

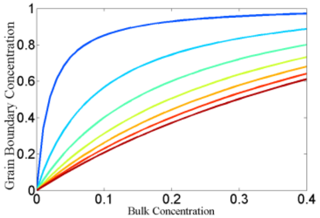
Grain Boundary Set Up

- 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
    - …

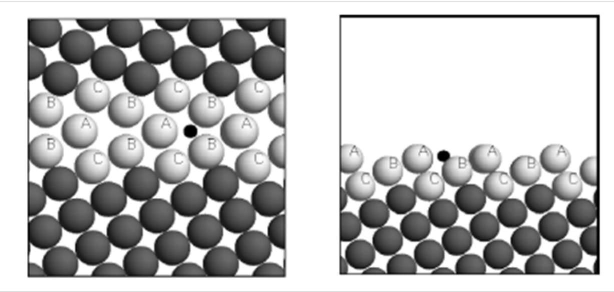
Site of Substitutional Impurity		Cr
Site A	boundary	−0.220
	surface	−0.560
	E_{surf}-E_{bound}	−0.340
Site B	boundary	−0.170
	surface	−0.560
	E_{surf}-E_{bound}	−0.390
Site C	boundary	−0.100
	surface	−0.340
	E_{surf}-E_{bound}	−0.240



E_s= -0.16 eV



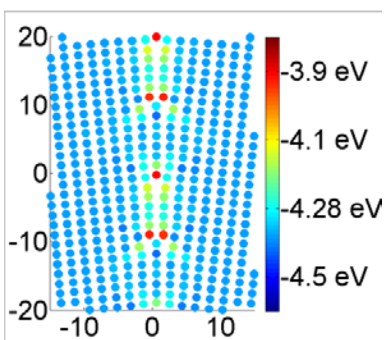
$$C_d = \frac{C \cdot e^{E_s/kT}}{1 - C + C \cdot e^{E_s/kT}}$$

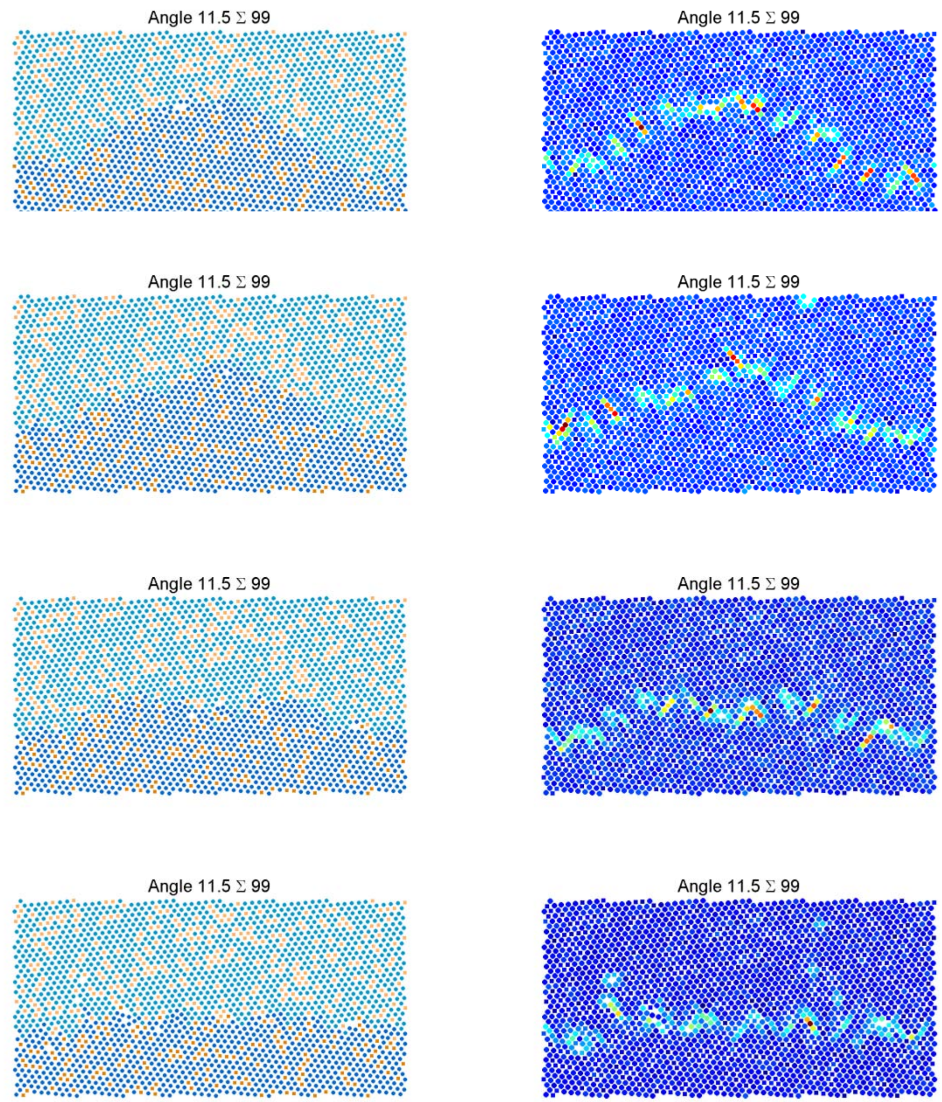


D. Farkas et al. Metallurgical and Materials Transactions A, 36A-pg 2067, (2005)

Simulation Results

- Case 11.5º
  - Low mobility
    - $M^* = 4\ E^{-9}\ m/s^2$
  - High Activation Energy
    - Q = 1.25 eV
  - Low grain boundary energy
    - $\gamma = 1\ J/m^2$
  - Grain boundary structure



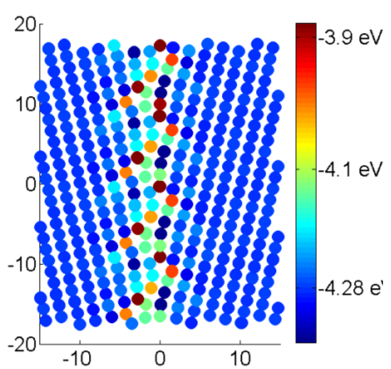


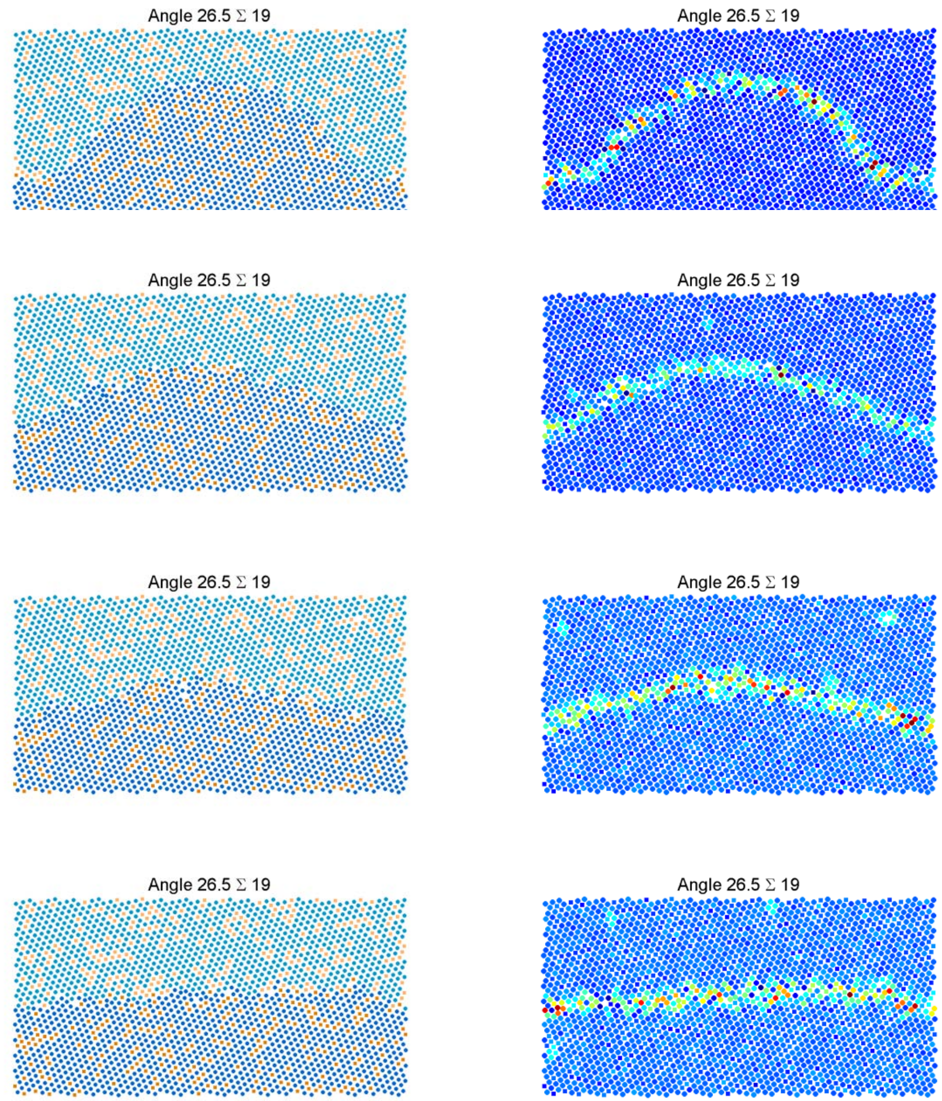
500 Pcs

Simulation Results

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

  - Grain boundary structure



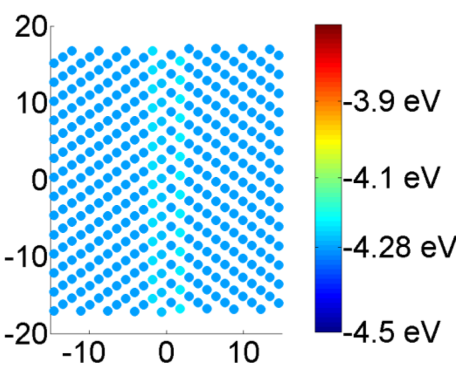


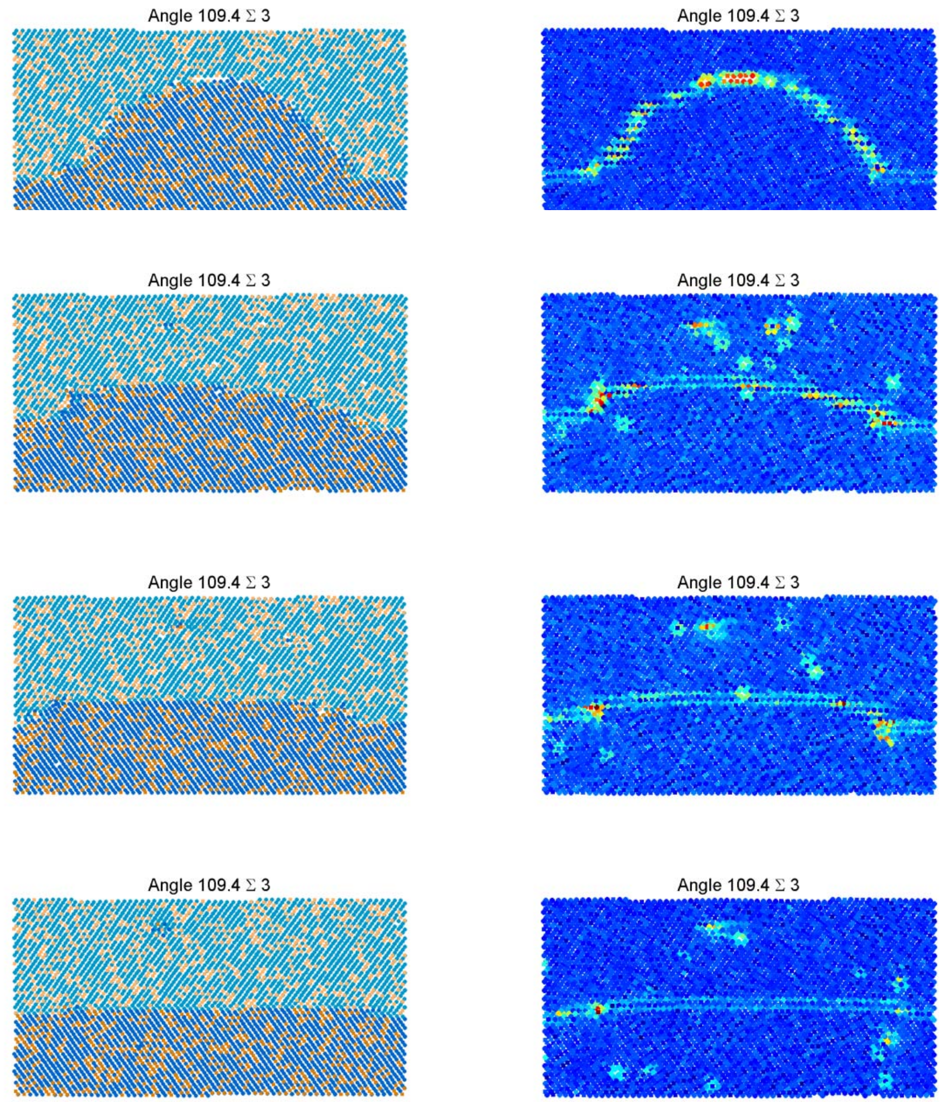
200 Pcs

Simulation Results

- Case 109º
  - Very High mobility
    - M* = 15 E^{-9} m/s^2
  - Very Low Activation Energy
    - Q = 0.27 eV
  - Low grain boundary energy
    - $\gamma = 0.7$ J/m^2

  - Grain boundary structure

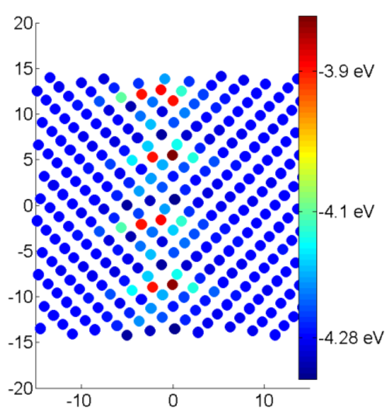


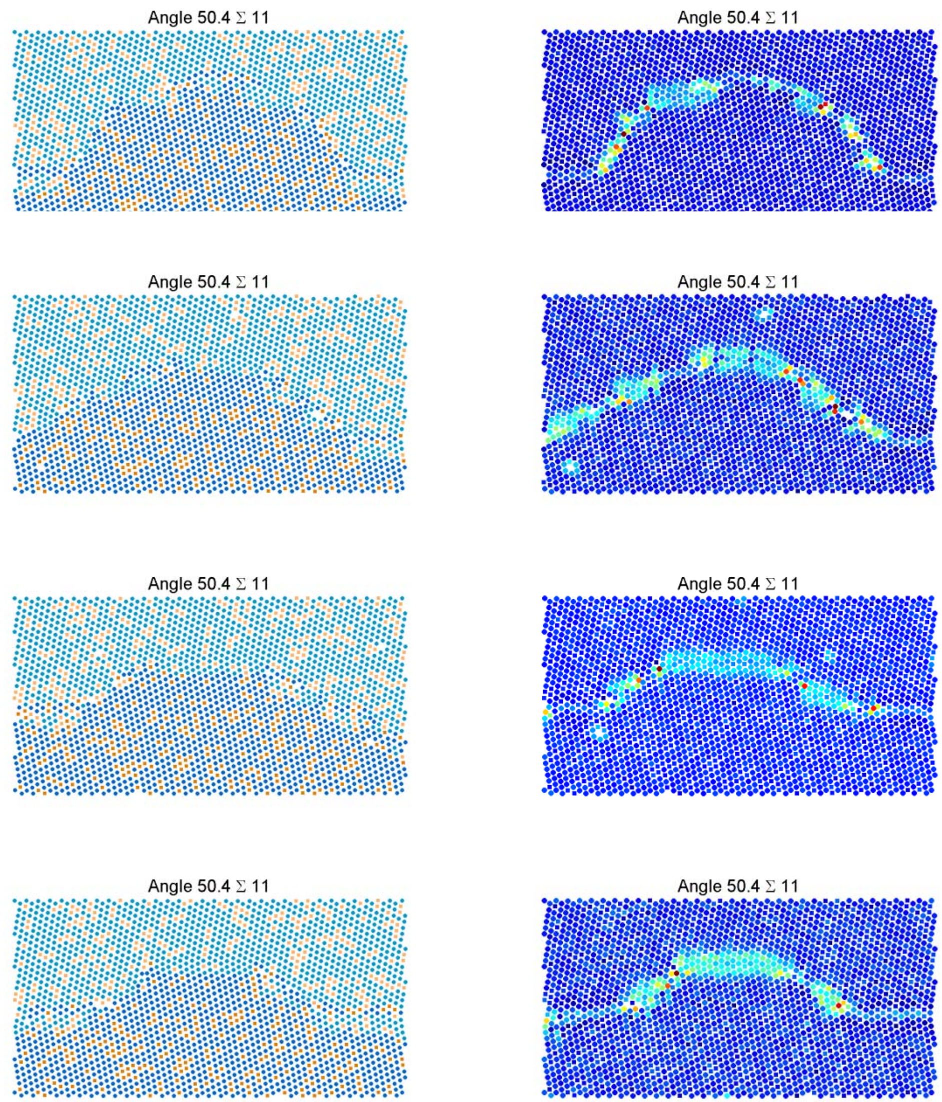


100 Pcs

Simulation Results

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



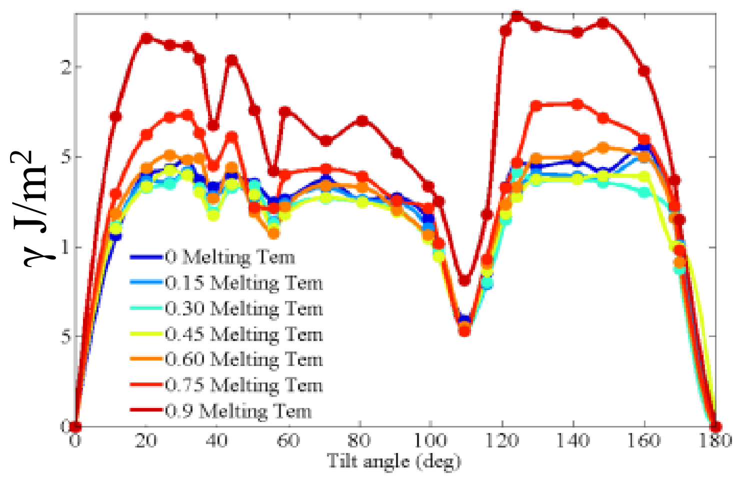


350 Pcs

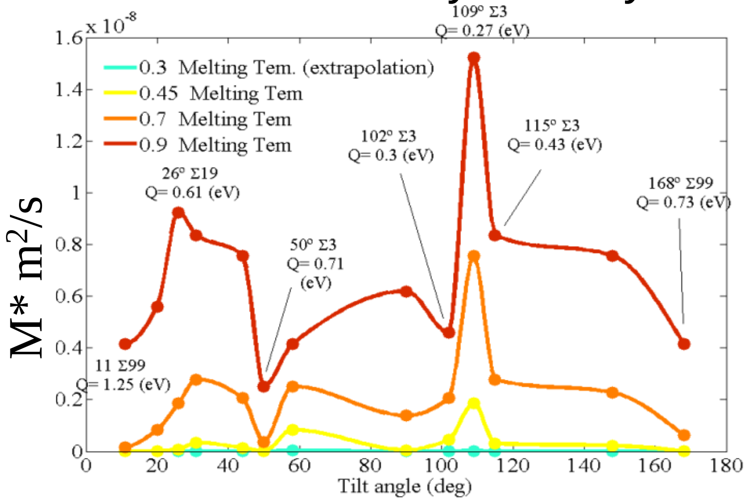
Simulation Results

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

<110> symmetric tilt
Grain boundary energy



<110> symmetric tilt
Grain Boundary Mobility



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

[1] C. Capdevila et al. ISIJ International, Vol. 43 (2003), No. 5, pp. 777–783

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 that HAGB
- But LAGB / HAGB classification is not enough to classify the mobility of a boundary
  - Configuration of atoms affect mobility as well as affects grain boundary energy
  - Low energy in HAGB has very high mobility
  - Some HAGB behave as LAGB
- I 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

[1] C. Capdevila et al. ISIJ International, Vol. 43 (2003), No. 5, pp. 777–783