Structure and Stability of Grain Boundaries in Iron

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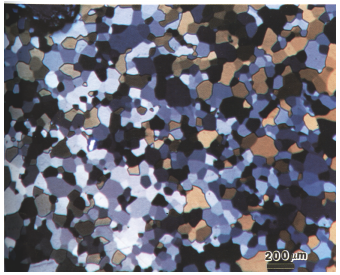
Multiscale Modeling of Real Materials
27th Max Born Symposium
17th - 20th September 2010
Wrocław • Poland

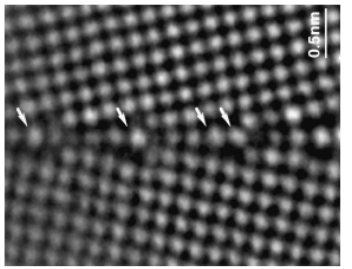
Outline

- Motivations
- Methods
- Results
- Conclusions

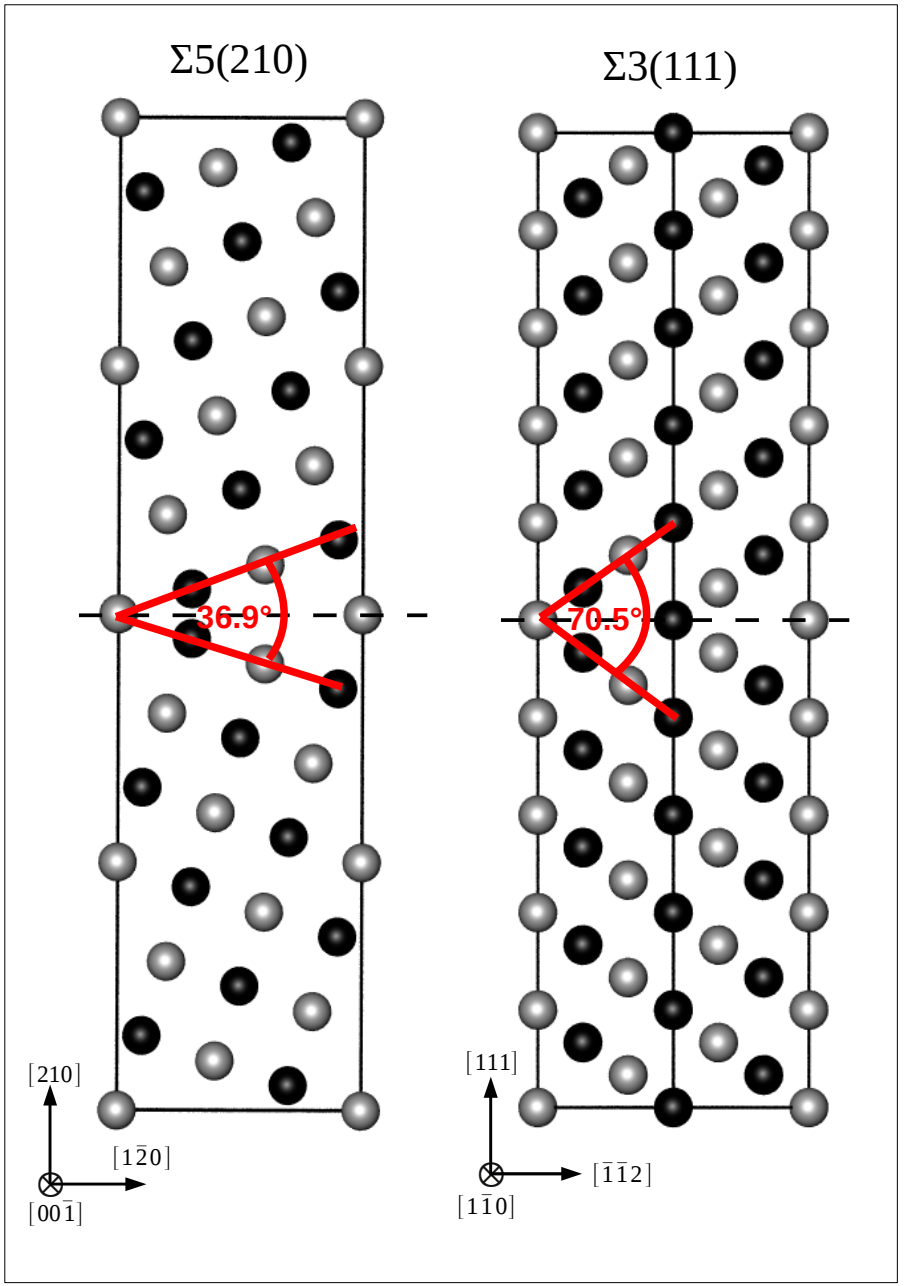
Motivation



- Fe and its alloys: one of the most popular materials
- Real materials: grains, grain boundaries and interfaces
- Fe-Cr – promising system for nuclear applications
- Vacancies or/and Cr segregation/depletion: mechanical and corrosion properties of materials are not clear from experiment
- *ab initio* DFT calculations: ∑5(210) and ∑3(111) one configuration
- Molecular Dynamics: ∑5(210) → 5 different configurations
- ∑5(210): geometry from DFT stable in MD
- Verification of MD geometries by DFT
- Vacancies and impurities at GBs



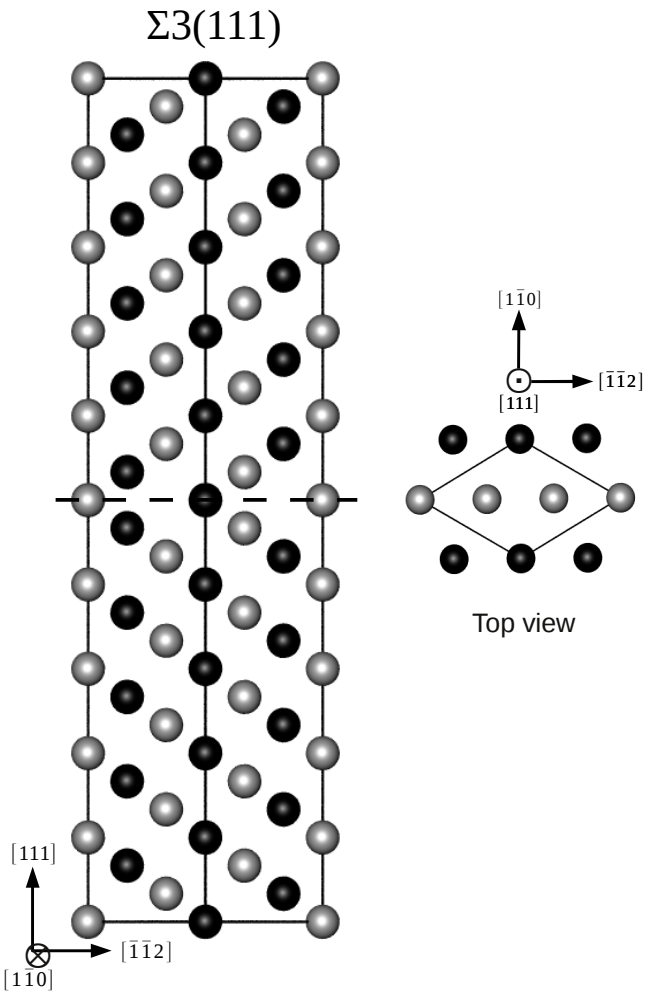
Methods

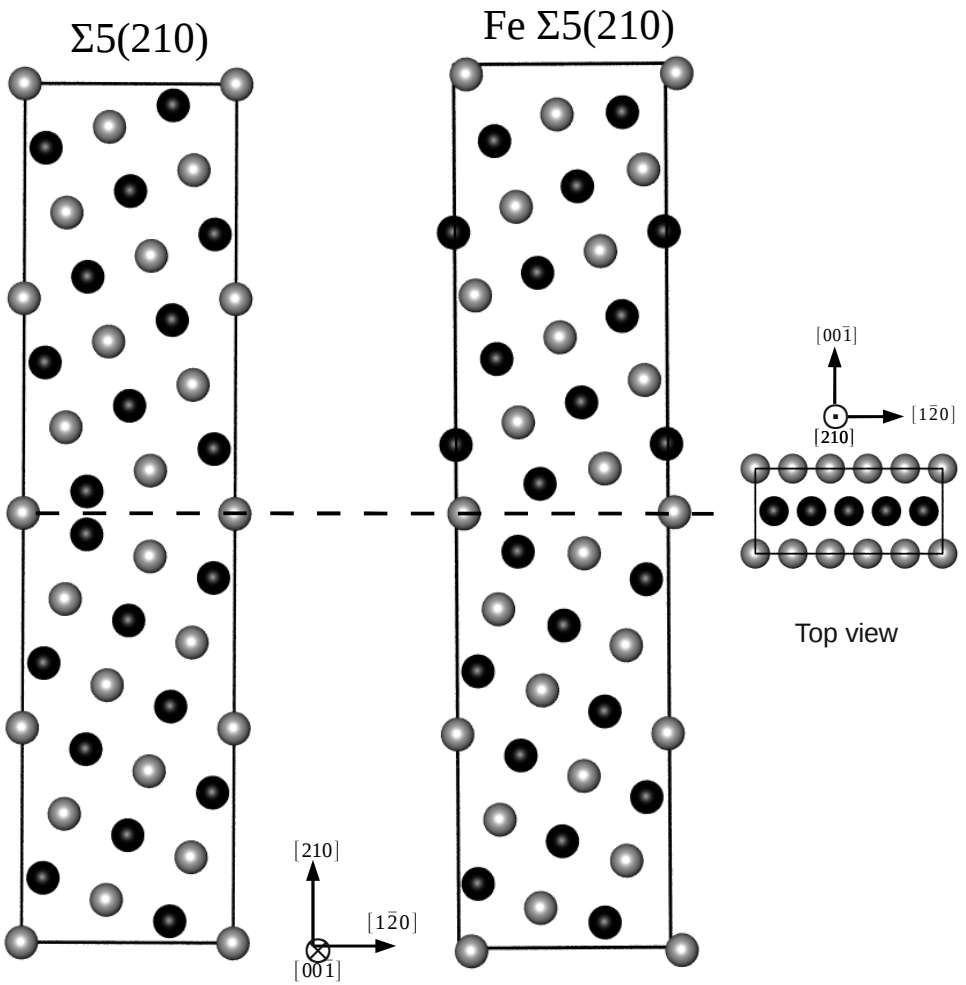


- Tilted grain boundaries ∑5(210) and ∑3(111).
- Supercells, periodic conditions
- *ab initio* DFT calculations
  - VASP
  - GGA – PW91 and PBE
  - spin-polarised
  - supercells (40 and 30 atoms)
  - full relaxation
- Molecular Dynamics (MD)
  - boxes of 8400 and 1728 atoms
  - interatomic potential of P. Olsson et al. Phys. Rev. B 72, 214119 (2009)
  - damped MD (0 K)

DFT calculations

E. Wachowicz et al., Phys. Rev. B, 81, 094104 (2010).





- symmetric
- E_{GB} = 1.57 J/m^2

- shift ~0.6 Å in [1$\bar{2}$0] direction
- E_{GB} = 2.00 J/m^2

Fe ∑5(210): DFT and MD

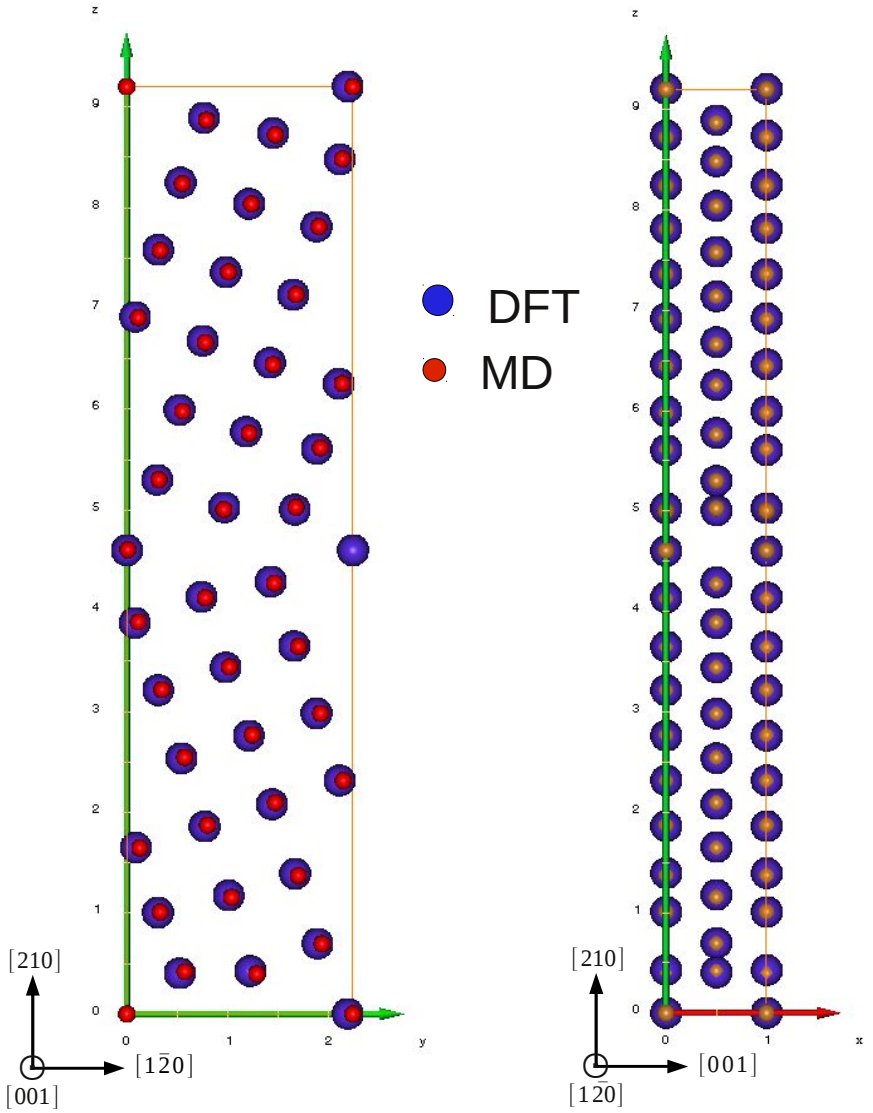


Fig. *Different side views of Fe Σ5(210) GB geometry from DFT and MD*

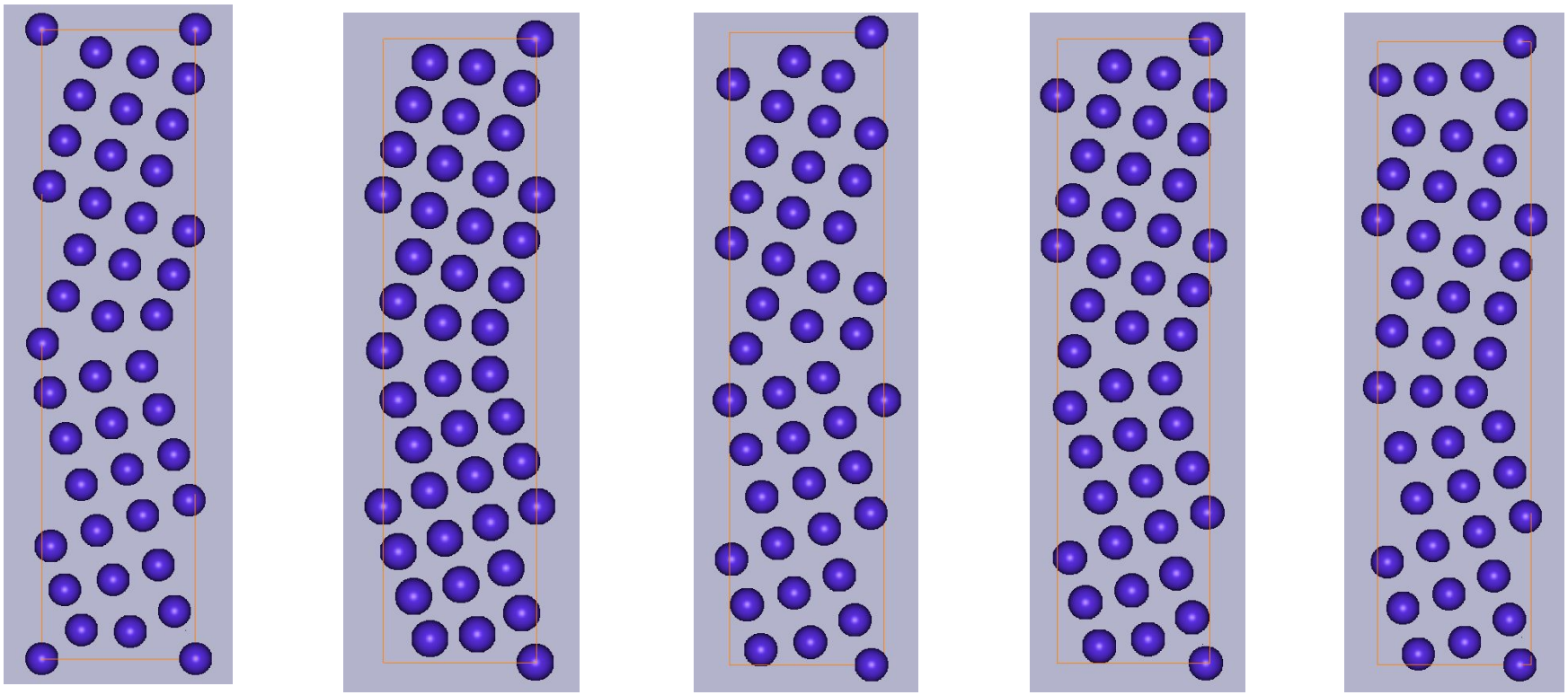
- Geometry from DFT is the same as from MD (0 K).
- GB energy:

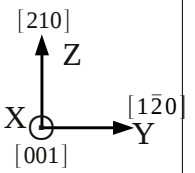
  DFT: 2.00 J/m^2
  MD: 1.42 J/m^2

Molecular Dynamics

- Fe ∑5(210): 5 different, stable structures

Initial shifts	cI (0;0;0)	cII (0.28;0;0)	cIII (0;1.14;0)	cIV (0.28;1.14;0)	cV (0;-1.71;0)
E_{GB}:	1.42 J/m^2	1.26 J/m^2	1.54 J/m^2	1.12 J/m^2	1.64 J/m^2





GB energy order: $E_{GB}^{cIV} < E_{GB}^{cII} < E_{GB}^{cI} < E_{GB}^{cIII} < E_{GB}^{cV}$

DFT calculations of MD configs.

Configuration	GB energy (J/m^2) MD	DFT
cI	1.42	2.00
cII	1.26	1.75
cIII	1.54	2.02
cIV	1.12	1.66
cV	1.64	→ cI

MD: $E_{GB}^{cIV} < E_{GB}^{cII} < E_{GB}^{cI} < E_{GB}^{cIII} < E_{GB}^{cV}$

DFT: $E_{GB}^{cIV} < E_{GB}^{cII} < E_{GB}^{cI} < E_{GB}^{cIII}$

- Configrations cI-cIV confirmed to exist in $ab\ initio$
- Interatomic potential apllied in MD describes very well interactions at GBs

MD and DFT order: $E_{GB}^{cIV} < E_{GB}^{cII} < E_{GB}^{cI} < E_{GB}^{cIII}$

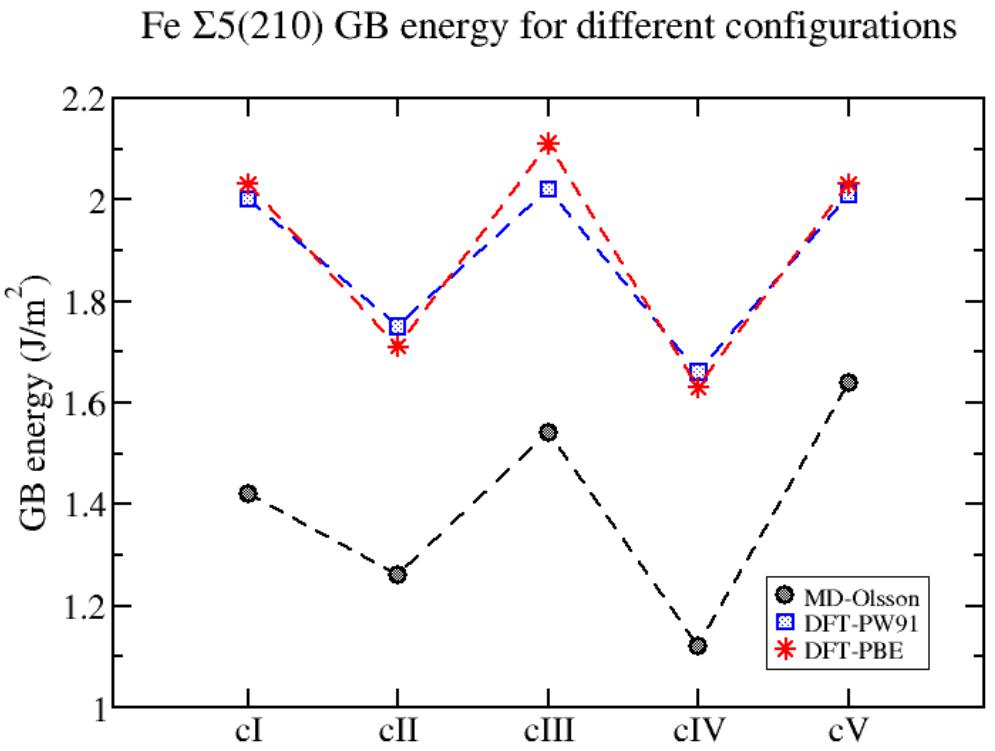
DFT: GGA PW91 and PBE XC

Configuration	GB energy (J/m^2) PBE	PW91
cI	2.03	2.00
cII	1.71	1.75
cIII	2.11	2.02
cIV	1.63	1.66
cV	→ cI	→ cI

DFT order: $E_{GB}^{cIV} < E_{GB}^{cII} < E_{GB}^{cI} < E_{GB}^{cIII}$

- Exchange-correlation does not influence energies and structures

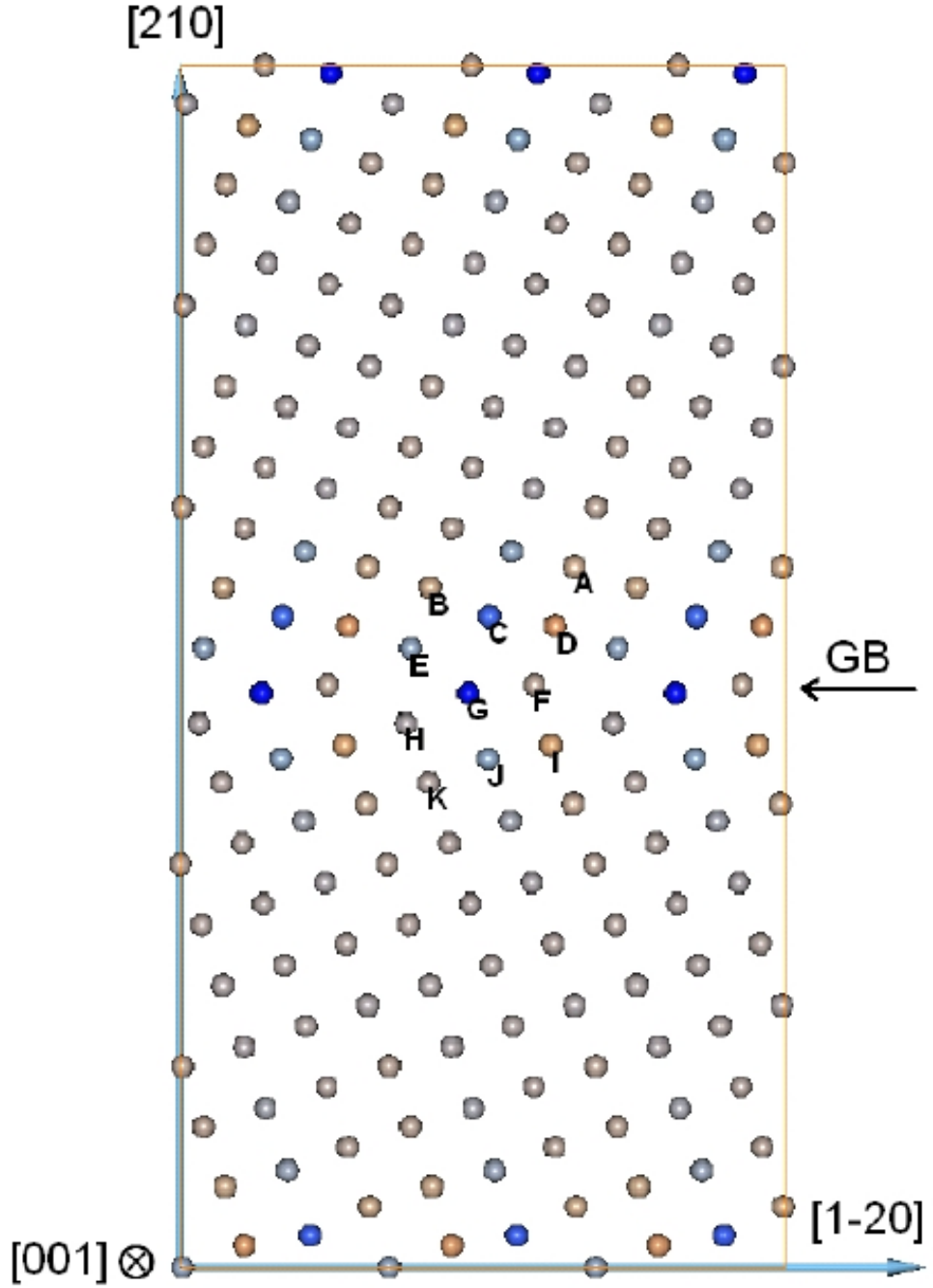
GB energy from DFT and MD



- General trend of GB energy is the same in DFT as in MD, most stable cIV configuration
- For symmetric ∑3 (111) configuration: E_{GB} (MD) = 1.31 J/m^2 , E_{GB} (DFT) = 1.57 J/m^2

Vacancies and Cr at ∑5(210) from MD

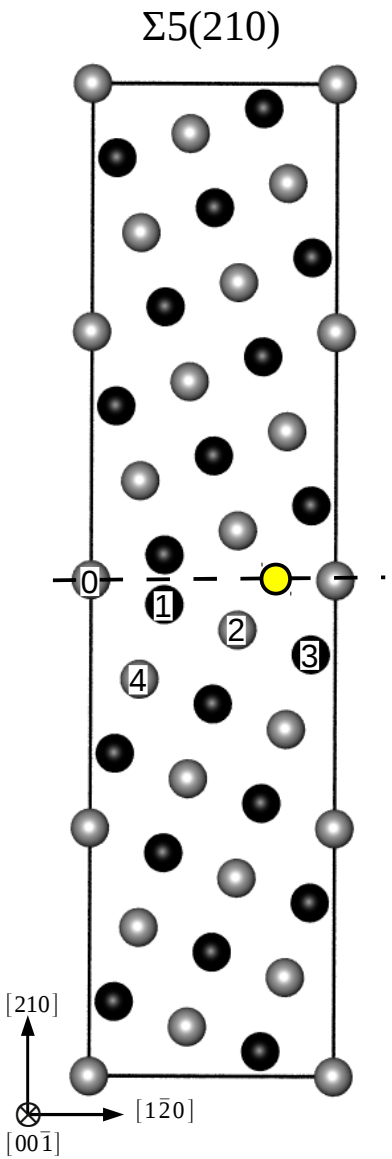
position	Binding energy [eV] E_b(V)	E_b(Cr)
D	+0.41	-0.05
E	+0.29	-0.07
F	+0.49	-0.11
G	-0.05	+0.27

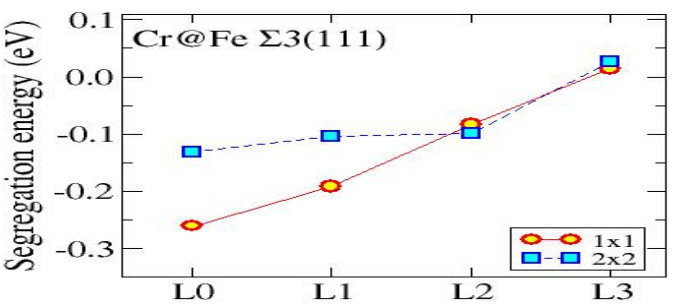


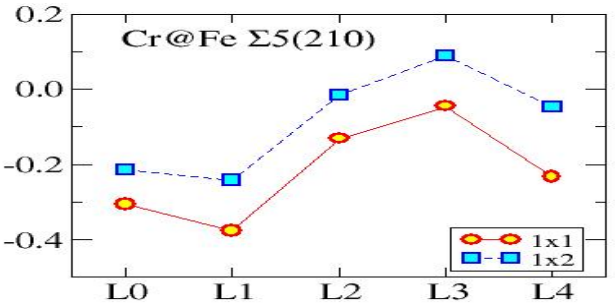
- Vacancies prefer sites near GB but not certain at the boundary (G)
- Cr atoms can be bound to certain positions at the GB
- Confirmation by means of *ab initio*: work in progress .....

Cr at Fe GBs

E. Wachowicz et al., Phys. Rev. B, 81, 094104 (2010).







- Cr segregates at both considered grain boundaries
- Cr enhances cohesion of Fe Gbs

SUMMARY

- We found most stable geometries for selected grain boundaries in Fe
- Very good agreement between DFT and MD results
- *Ab initio* calculations confirmed quality of potential describes interatomic interactions in MD simulations
- Cr additions prefer sites at GBs in Iron and are cohesion enhancers
- Vacancies prefer sites near boundaries (MD)
- Additional DFT results needed for Cr and vacancies at GBs (work in progress)