ALEMI Workshop, 25 May 2009

Bridging the Gap

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A New Process Model for Steels by Modelling Across Different Length Scales

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A Canadian Modelling Initiative

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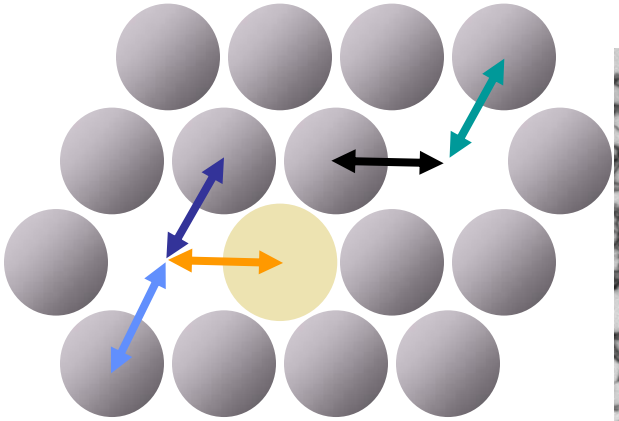
Length Scales

Atomistic:

10^{-9} – 10^{-10} m

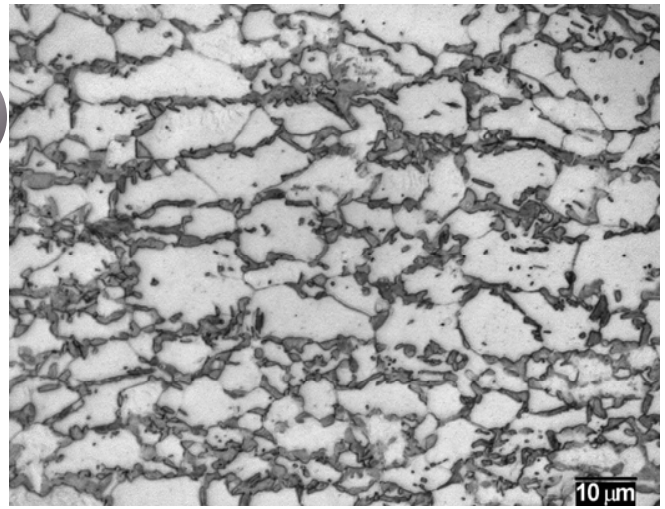
Microstructure evolution associated with motion of atoms



Mesoscale:

10^{-6} – 10^{-4} m

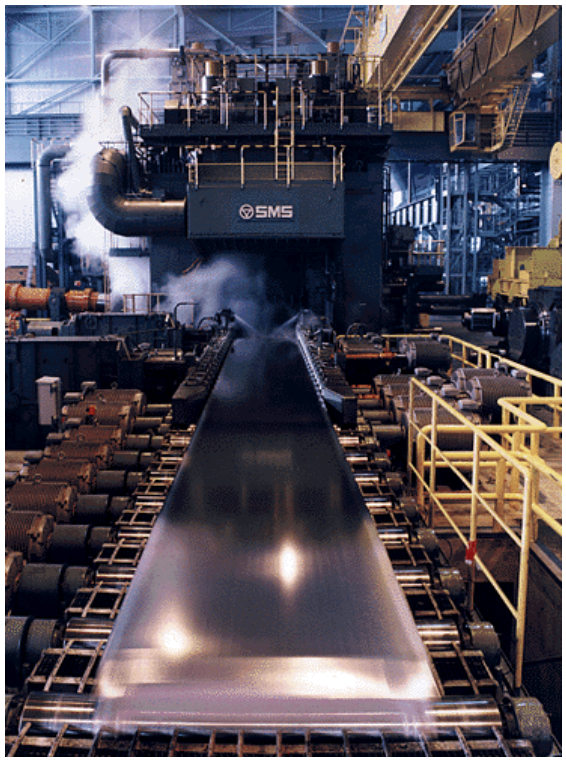
Scale of microstructure



Macroscale:

0.01 – 10 m

Size of industrial sheet, coil or laboratory sample



Process Models

Process Models – formulated on Macroscale

e.g. JMAK for fraction transformed

$$X = 1 - \exp\left\{ -\frac{1}{d_\gamma^{\,m}} \left(\int_T^{T_s} \frac{\beta(T)^{1/k}}{\varphi(T)} dT \right)^k \right\}$$

Model parameters – depend on phenomena on Atomistic Scale

e.g. for interface-controlled reaction JMAK rate parameter function of interface mobility

$$\beta = MG$$

interface mobility affected by alloying elements (solute drag)

$$M = \left(\frac{1}{M_{pure}} + \alpha_m c_m \right)^{-1}$$

➡ Solute drag parameters: E_o and D_b/δ

➡ **Rigorous modelling approach – Need to connect atomistic scale to macroscale**

Unknown Quantities

Adjustable parameters → ***M*, D_b/δ and E_o**

Can we determine all or some of these parameters from atomistic simulations?

- **M, Mobility of pure interface** (Molecular Dynamics)
- $D_b=D_o\exp(-Q_b/kT)$, Diffusivity of solute across interface (Molecular Dynamics?)
- **Q_b, Activation energy of interfacial solute diffusion** (Density Functional Theory)
- **E_o, Binding energy of solute to interface** (Density Functional Theory)

Length Scales and Project Flow

Atomistic:

DFT (density functional theory): ab-initio calculation of binding (E_o) and activation energies (E_A) of solutes at α-γ interface

MD (molecular dynamics): Use DFT results to build suitable potentials for simulations of diffusion (D_b) across and mobility (**M**) of α-γ interface

Mesoscale:

PFC (phase field crystal): Provide linkage from atomistic to continuums modelling using MD length scale and PFM time scale, translate interaction potentials to two-point correlation function (c_2)

PFM (phase field model): Use DFT/MD/PFC (c_2) results for binding energy (E_o), interfacial diffusion (D_b) and mobility (**M**) to simulate **solute drag** and overall transformation kinetics

Macroscale:

JMAK (Johnson-Mehl-Avrami-Kolmogorov): Translate PFM **solute drag** model into suitable **JMAK rate parameters** for overall **transformation model**

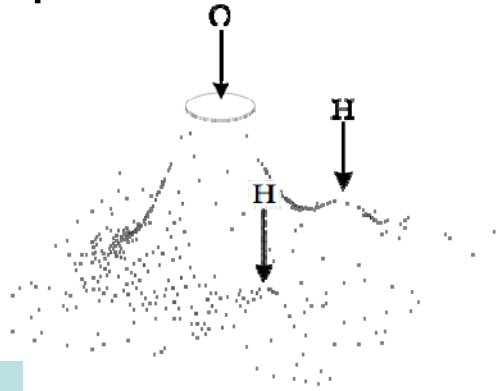
Validation Experiments: **Validate transformation model** with experimental data

Density Functional Theory

Electron Density: $\rho(\vec{r})$ Probability to find electron at a given point in space and time

Hohenberg and Khon :

$$\rho(\vec{r}) \xrightarrow[F(\rho(\vec{r}))]{} E_{Total}$$



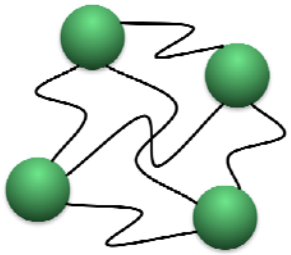
If the form of functional F is known, one can immediately find the total energy of the system for any given charge density distribution.

$$E[\rho] = T[\rho] + E_{ee}[\rho] + E_{en}[\rho]$$

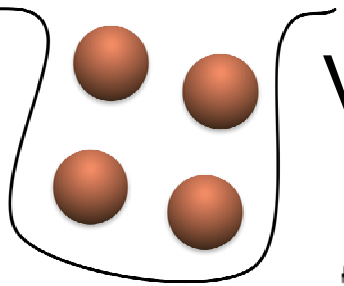
Kinetic energy + Potential Energy

Density Functional Theory

Khon and Sham:



$\rho_{int} = \rho_{nonint}$



V_{eff}

$$\rho(\vec{r}) = \sum_{i}^{N} | \phi_i(\vec{r}) |^2$$

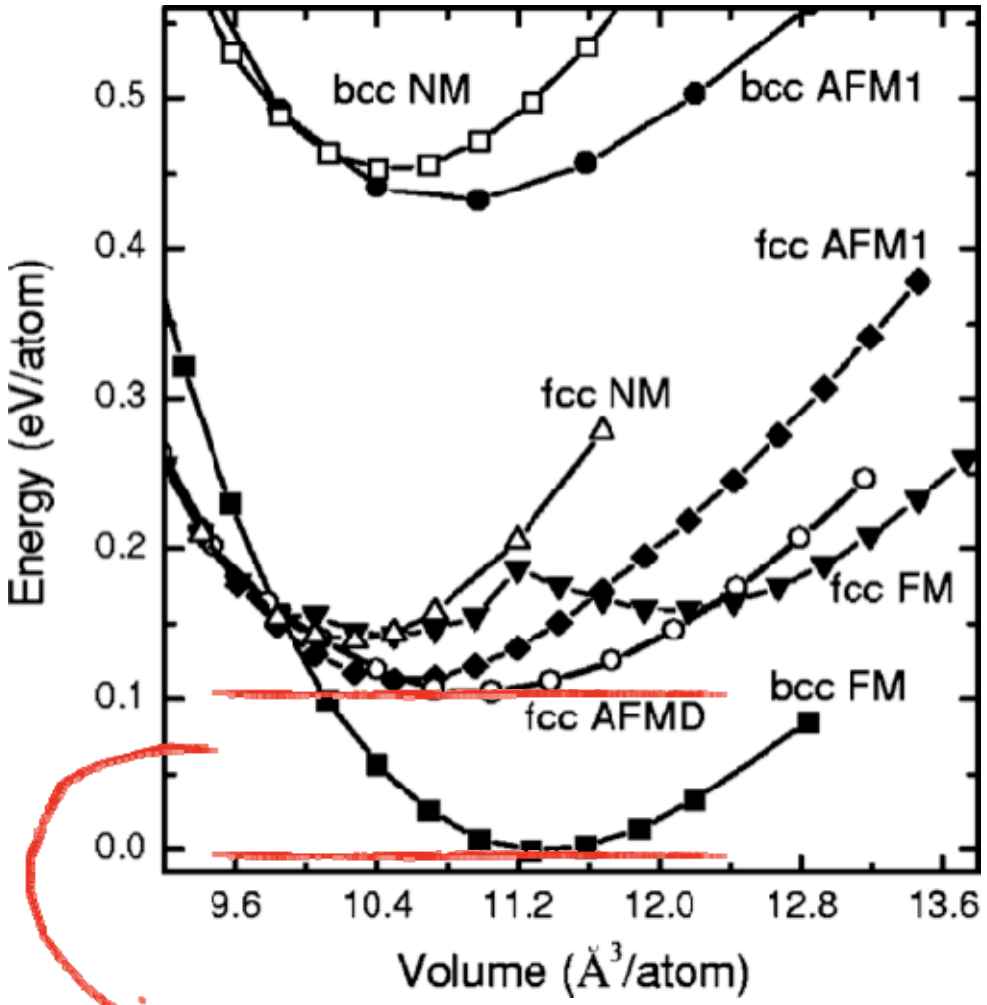
Replace system of interacting electrons with system of non interacting electrons with the same electron density.

$$(-\frac{1}{2}\vec{\nabla}^2 + \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}' + V_{xc} + V_{ext})\phi^n(\vec{r}) = \epsilon^n \phi^n(\vec{r})$$

V_{eff}

- Need to find approximation for V_{xc} using theory of interacting electron gas (LDA, GGA etc)
- Ground state theory (T = 0 K)
- Currently: DFT simulations with system size < 1000 atoms

Density Functional Theory



0.1eV = 1160 K = 887 °C

Fe bcc / fcc – bulk calculations

	a (Å)	B (GPa)	M (μ_B)
DFT	2.83	174	2.20
Exp.	2.86	168	2.22

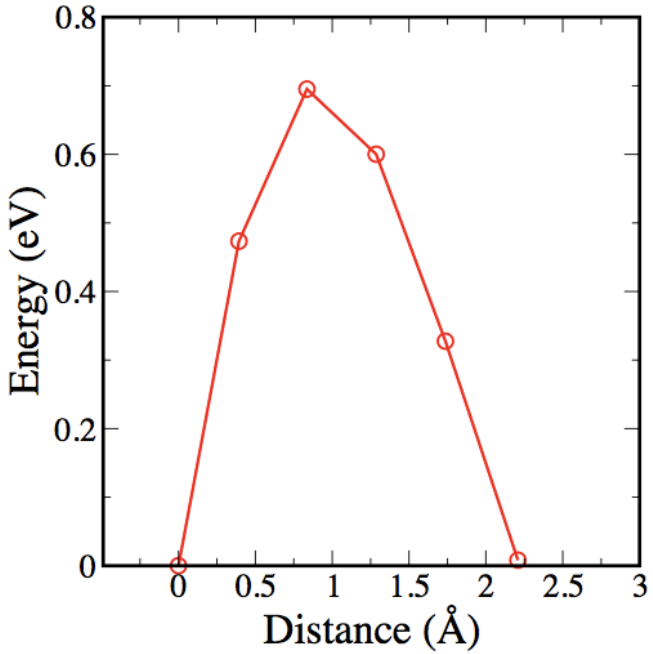
~1% error in a

D.E. Jiang and E.A. Carter, PRB **67,** 214103 (2003)

Self Diffusion in bcc Fe

Calculation details:

- Ferromagnetic spin arrangement
- Supercell: 3x3x3 (54 atoms)
- Periodic boundary conditions
- NEB to find minimum energy path

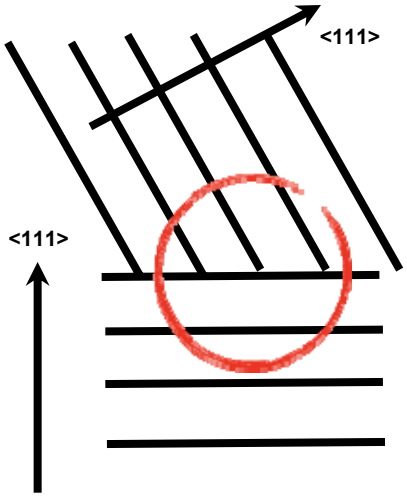


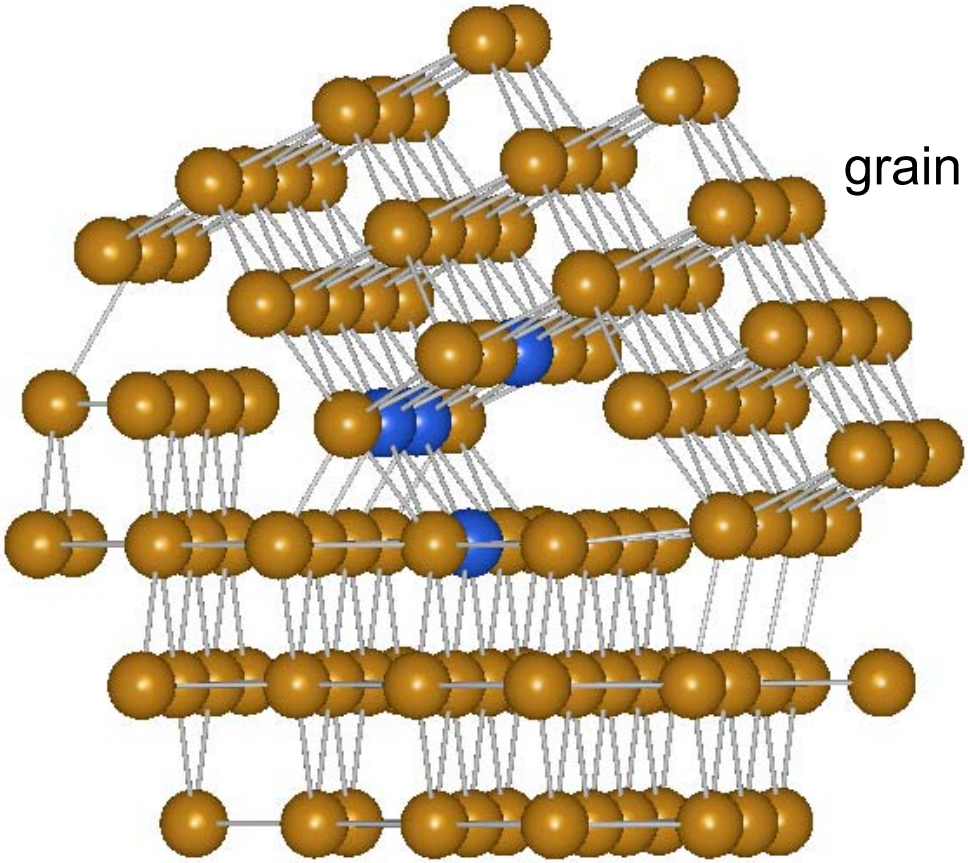
Results:

- Migration energy E_M=0.69eV
- Vacancy Formation energy E_{vf}=1.88eV
- Activation energy E_A=2.57eV

experiment : 2.7eV

Interfaces in DFT Simulations



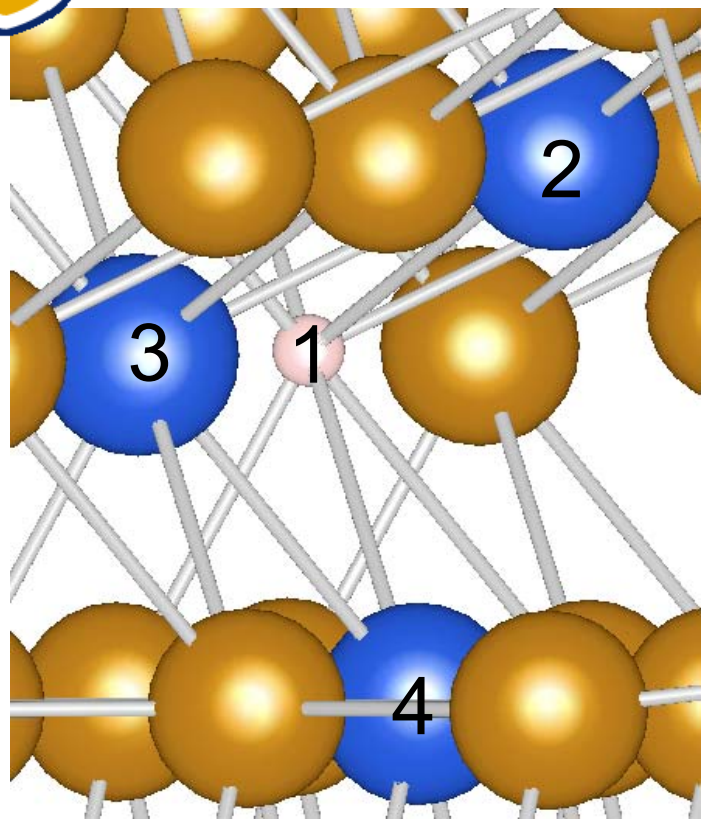


grain boundary in bcc-Fe

Cluster of 115 atoms

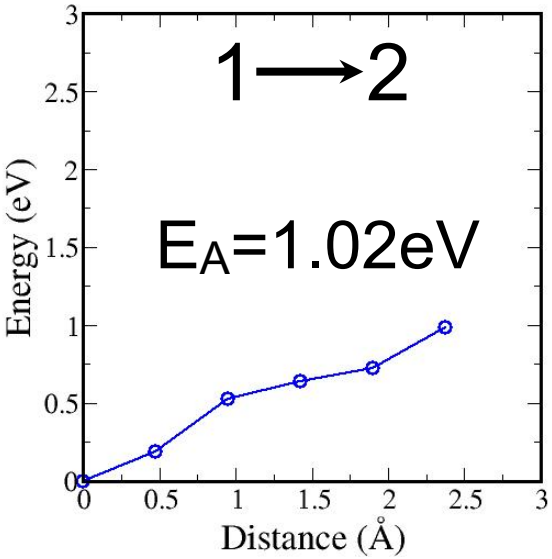
- **Cluster (size effects!)**
- **Periodic boundary conditions (special boundaries)**
- **Embedded clusters?**

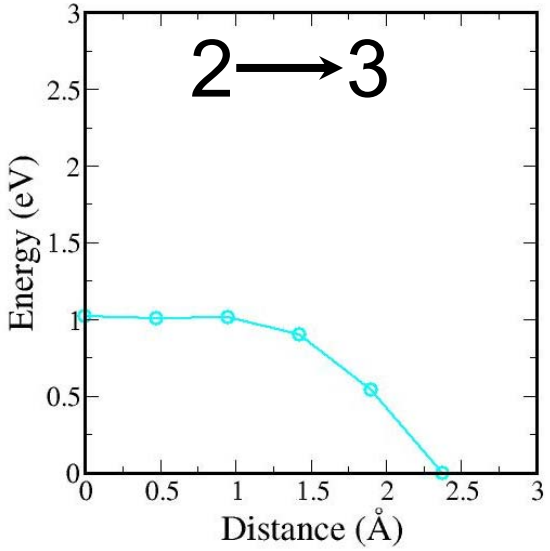
Grain Boundary Self Diffusion

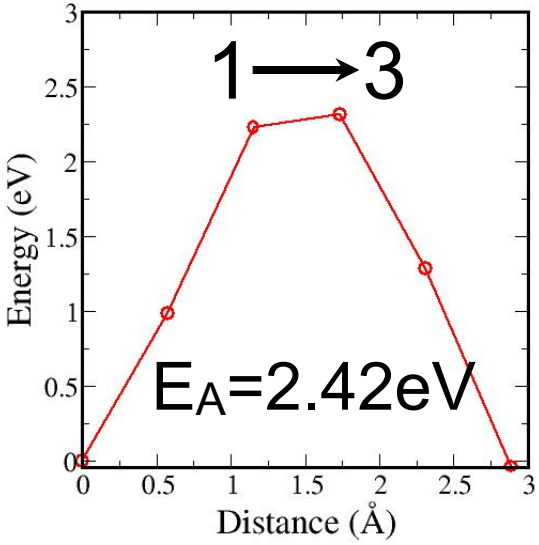


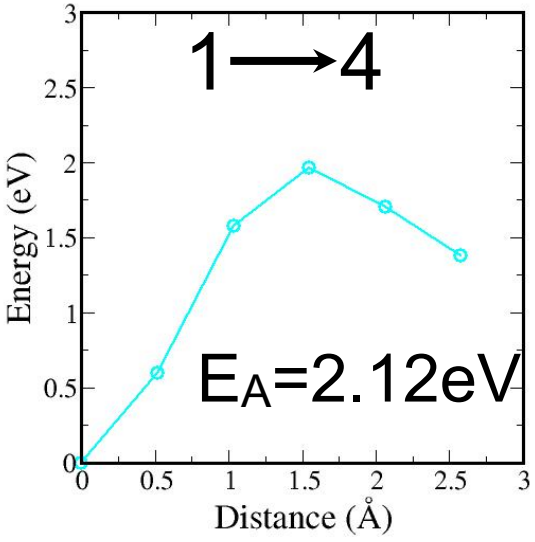
Vacancy Formation energy at position 1

E_{vf}=0.02eV









DFT simulations for α-γ interface

General issues with interface problems

- size and boundary conditions of calculation domain
- multiplicity of calculations to determine representative values for binding and activation energies

Specific issues with α-γ interfaces in DFT

- bcc-Fe is ferromagnetic
- fcc-Fe is paramagnetic at transformation temperatures
- magnetic state of fcc-Fe at T=0K?
- assume fcc-Fe to be antiferromagnetic?
- currently no clear picture how to handle magnetism of fcc-Fe in DFT

Molecular Dynamics

Need suitable EAM potentials
– available for Fe, as well as C, P and Al in Fe

Mobility of the Austenite/Ferrite interface
for pure Fe and Fe-C from classical MD simulations
using several techniques

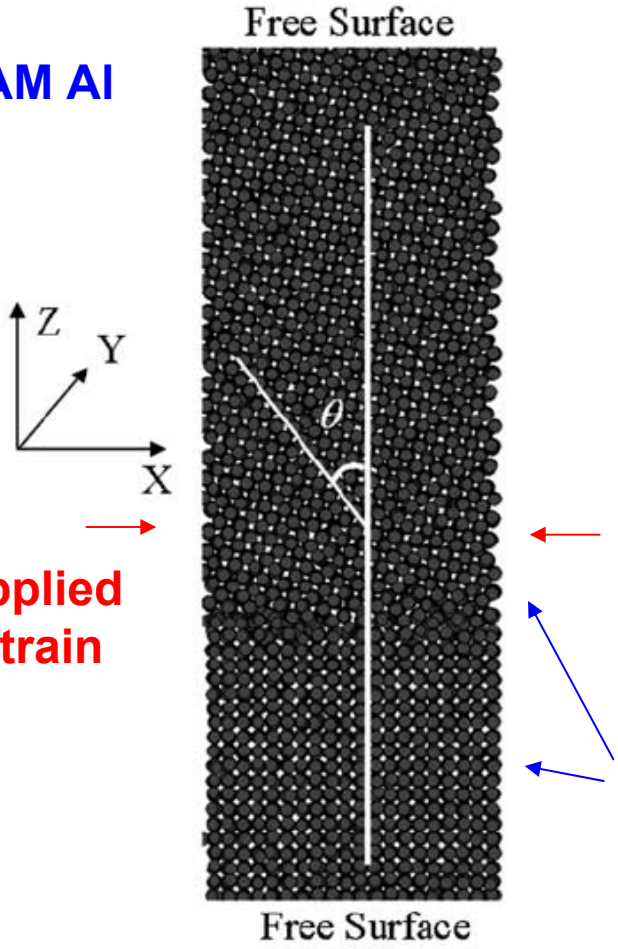
1) Applications of driving force

2) Fluctuations

Molecular Dynamics

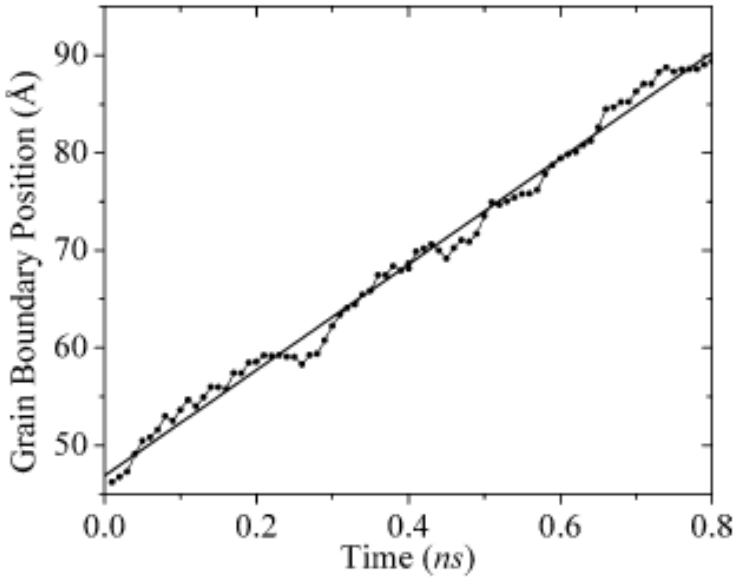
Driving Force: 1) Elastic Strain Energy

EAM Al



Applied Strain

Zhang, Mendelev, Srolovitz, Acta Mater., 52, 2569 (2004)

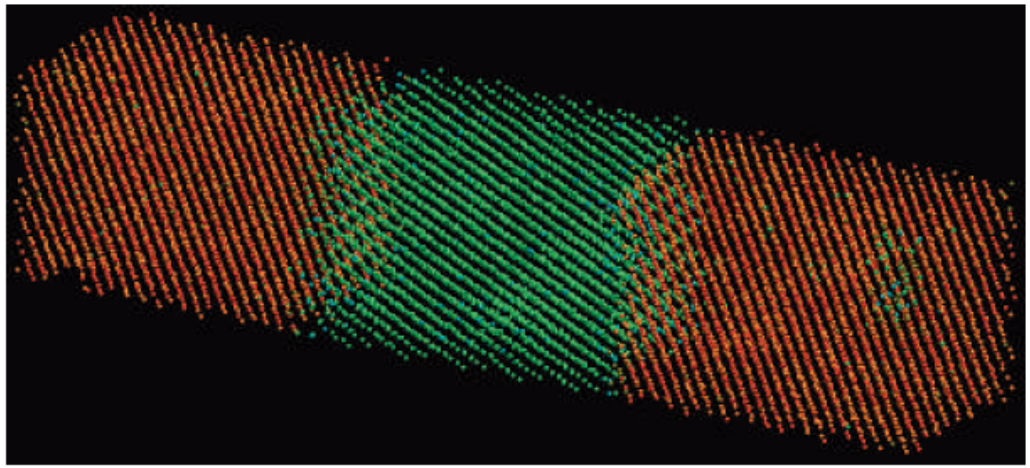


Anisotropy means $1/2\varepsilon_{ij}\sigma_{ij}$ is different in each grain

Molecular Dynamics

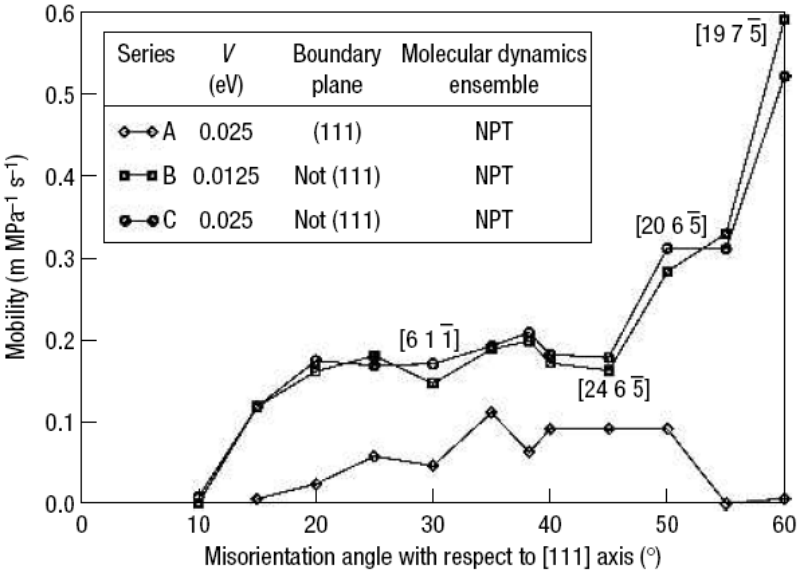
Driving Force: 2) Artificial

EAM Al



Janssens et al. Nature Matls., 5, 124 (2006)

Potential energy added to atoms based on the local orientation. Green high PE, red zero PE added



Conclusions and Future Work

- MD promising tool to determine mobility in pure Fe and Fe-C
- Does unrealistic driving pressure affect M?
- DFT in principle promising tool to determine solute drag parameters
- Magnetic state of fcc-Fe as fundamental issue for DFT simulations
- Systematic studies of solutes at bcc/bcc interfaces as intermediate step
- Translation of results of atomistic simulations into parameters for phenomenological models