2006-10

Heterogeneous precipitation of Cu in Fe-Cu alloys

Caro, M.

U.S. Department of Energy

A, Caro, M. Caro, "Heterogeneous precipitation of Cu in Fe-Cu alloys," IGRDM-13, Tsukuba, Japan October 15-20, 2006 , 19 p.
http://hdl.handle.net/10945/52660

UCRL-CONF-225781

Heterogeneous precipitation of Cu in Fe-Cu alloys

M. Caro, A. Caro

November 1, 2006

IGRDM-13
Tsukuba, Japan
October 15, 2006 through October 20, 2006

Heterogeneous precipitation of Cu in Fe-Cu alloys

IGRDM-13

15-20 October 2006

M. Caro, A. Caro

Chemistry and Materials Science
Lawrence Livermore National Laboratory

E. M. Lopasso (CABariloche-Argentina), B. Sadigh (LLNL), P. Turchi (LLNL),
D. Crowson (Virginia Tech.), P. Klaver (QUBelfast-UK), S. Srivilliputhur (LANL)
The summer students:
H. Dogo (Naval Postgraduate School), S. Garcia Gil (University of Barcelona), M. Gilbert (UKAEA)

UCRL-CONF-225781

This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

We are developing models and computational tools for alloys to understand radiation damage in nuclear materials

Motivation

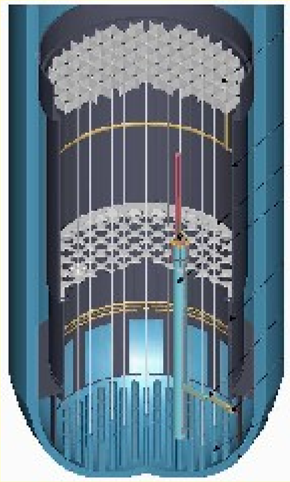
• Copper is found as an impurity in reactor pressure vessel steels

• Radiation induced Cu precipitation leads to changes in the microstructure and controls damage effects such as embrittlement and radiation hardening

Nuclear materials

Microstructural evolution of structural steels under irradiation

Reactor Pressure Vessel



www.tecnatom.es/english/catalogo

We investigate the formation of Cu precipitates in Fe-Cu alloys of low Cu concentration using :

• a classic potential that has been fully characterized thermodynamically

• a parallel Monte Carlo code with displacements that allows to perform simulations of heterogeneous precipitation

Classic interatomic potentials for MD / MC simulations in alloys

Models

Stage I

Understand what models predict

Stage II

Develop models that behave as desired …

Our objective is to relate *ab initio* energetics, alloy potentials, thermodynamics, and microstructures

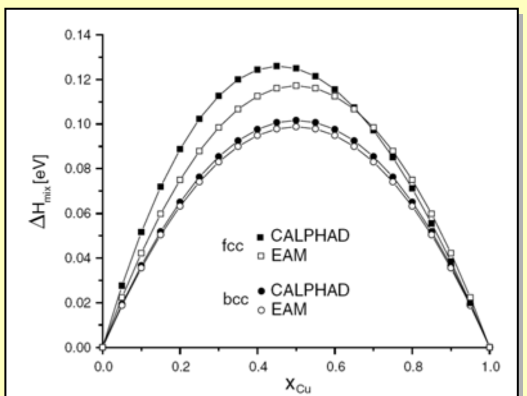
chemistry & materials science CMS

1

ab initio ⟺ potentials

- **A methodology to generate classic potentials able to reproduce formation energy of complex alloys**

JNM 349, 317 (2006)



Excess enthalpy of mixing at 0 K for both fcc and bcc FeCu solid solutions

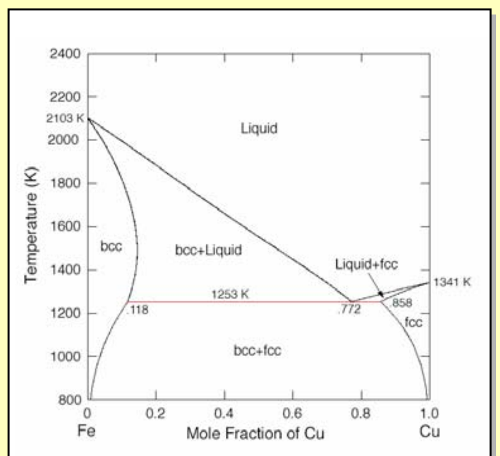
2

potentials ⟺ thermodynamics

- **A unique suite of codes to evaluate free energies:**

  an *entropy - meter*

Phys. Rev. B 66, 054201, (2002)
Phys. Rev. B 68, 214205, (2003)



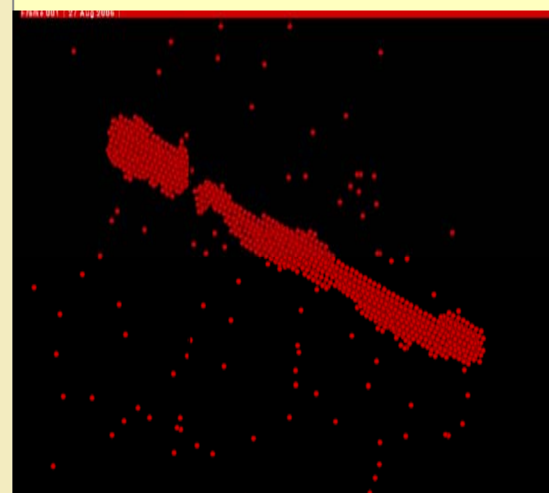
Phase Diagram of EAM FeCu

3

potentials ⟺ microstructure

- **A powerful massively parallel Monte Carlo code with displacements to study heterogeneous precipitation**

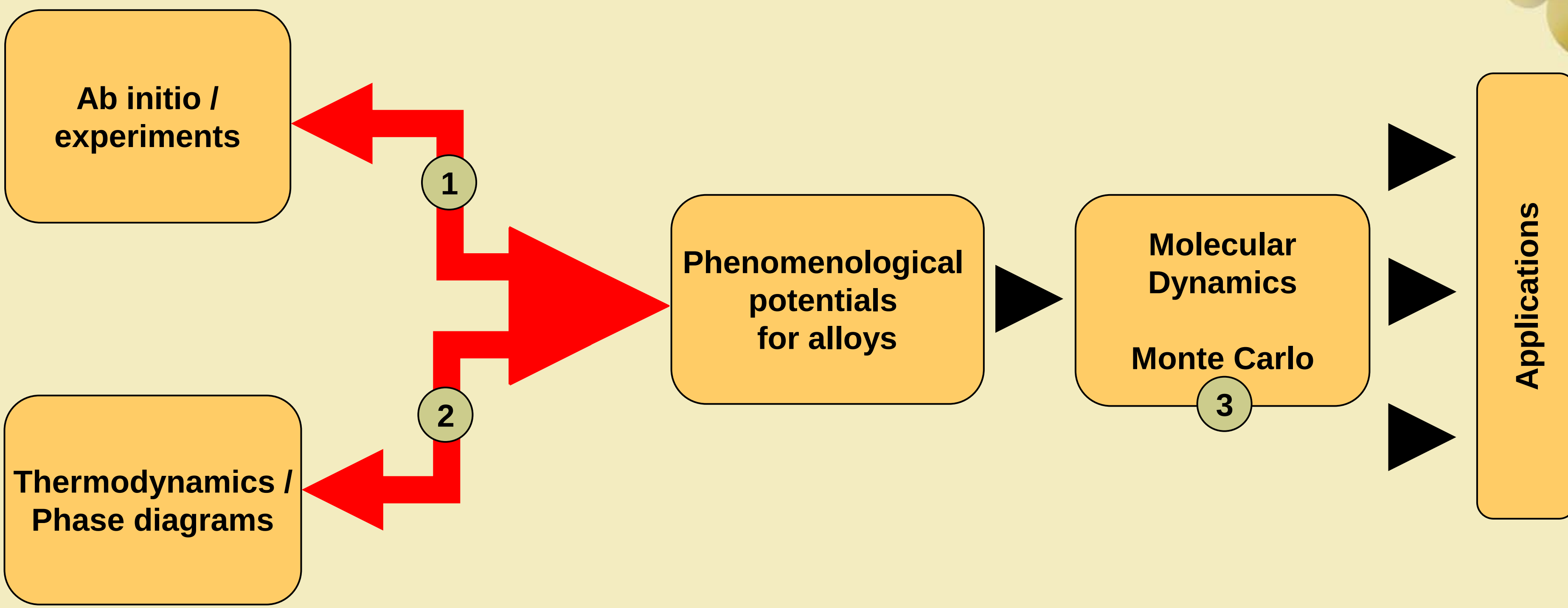
Appl. Phys. Lett. 87, 231904 (2005)



Cu precipitates on screw dislocation

We work on:

1. New approach to generate potentials for alloys
2. Thermodynamic package
3. Parallel Monte Carlo code w/displacements



② Computational Thermodynamics

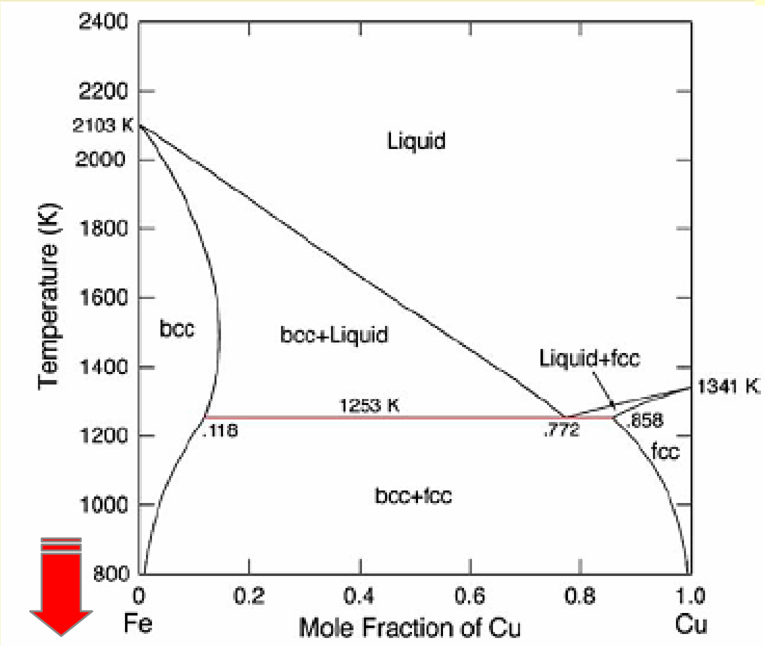
We evaluate free energies

$$F = -kT \ln\left(\int_{\Omega} \exp(-H(x))dx\right)$$

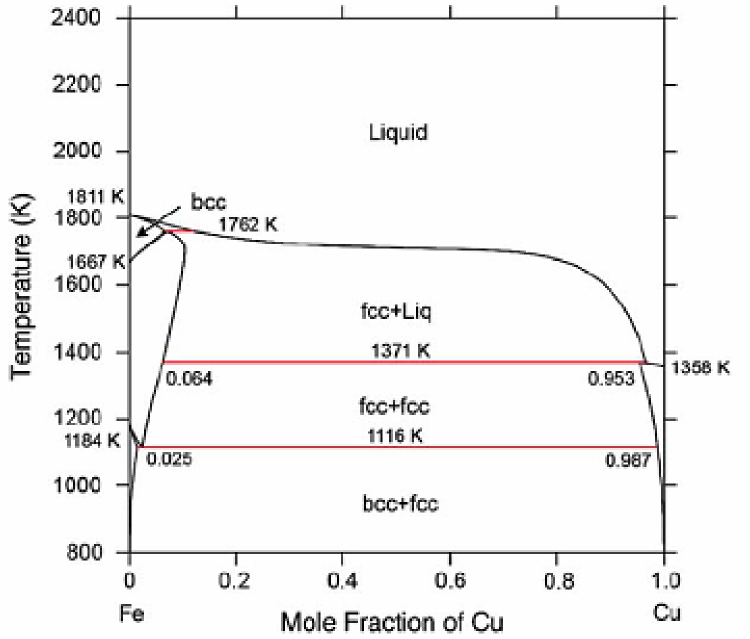
Switching Hamiltonians
Gibbs – Duhem integration
Gas expansion
…

Phys. Rev. **B 66**, 054201, (2002)
Phys. Rev. **B. 68**, 214205 (2003)
J. Nuc. Mat. **336**, 233 (2005)
J. Nuc. Mat. **349**, 317 (2006)

Phase diagram corresponding to
Ludwig-Farkas Fe-Cu EAM Potentials



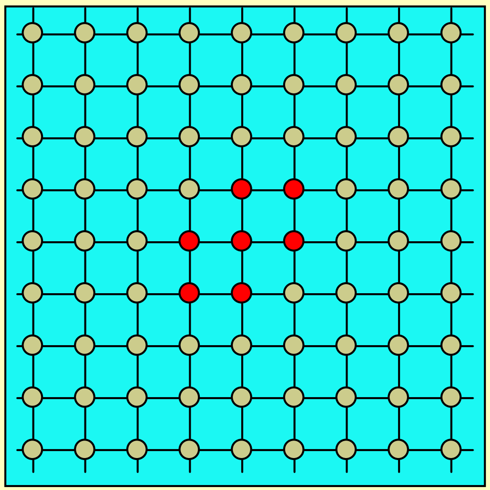
CALPHAD Fe-Cu Phase Diagram
Experiment



Region of nuclear interest

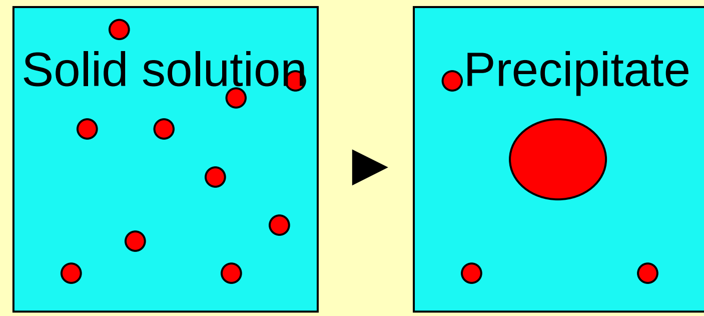
We developed a massively parallel displacement Monte Carlo code to predict microstructures

Lattice Monte Carlo



$\Delta G = -V\,\Delta E + A\,\gamma'$

Monte Carlo with displacements



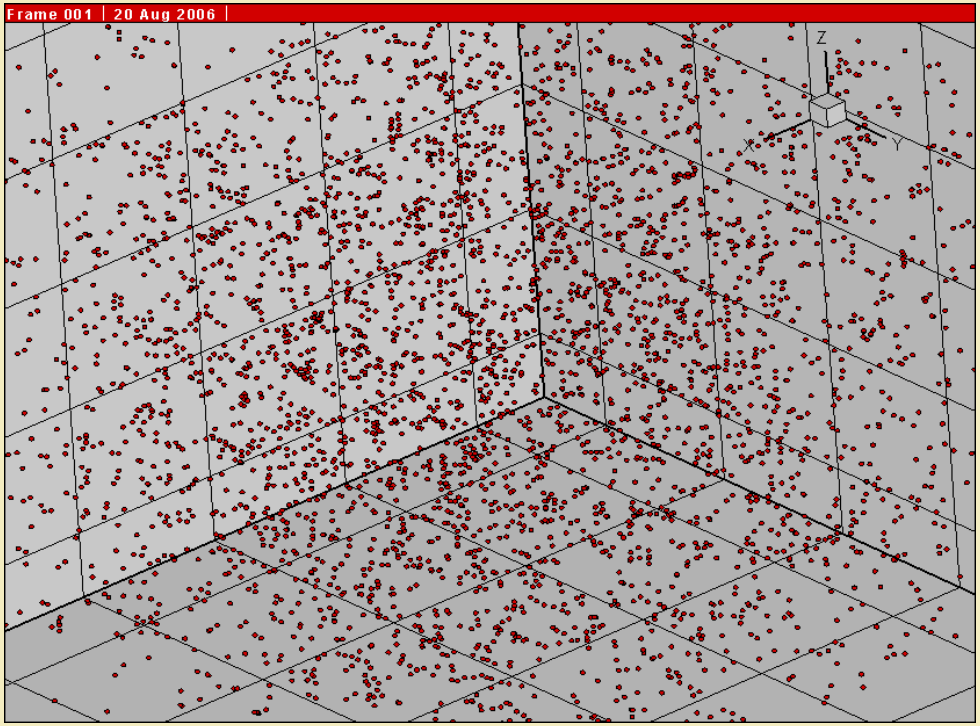
G_1 $\qquad$ $\Delta G = G\beta - G\alpha$

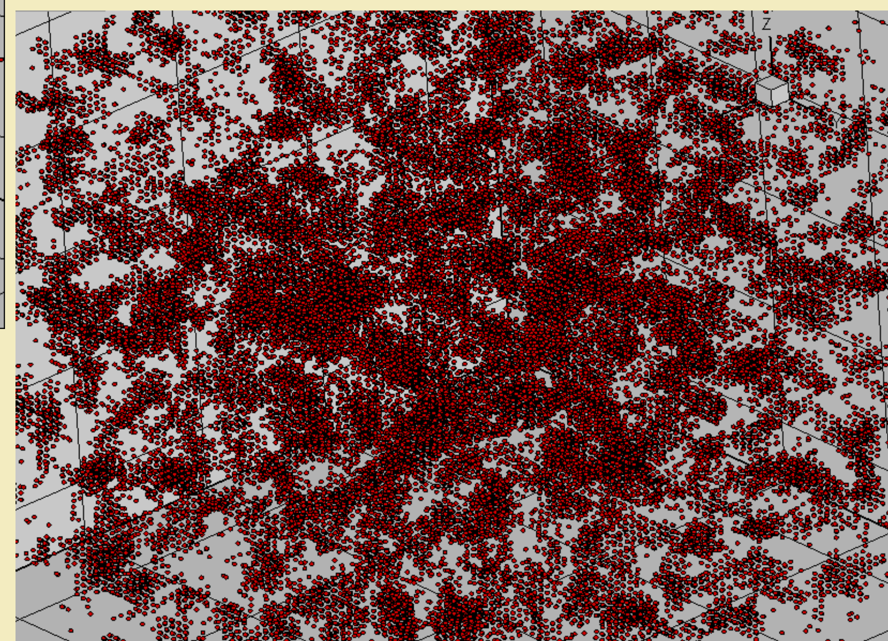
$\Delta G = -V\,(G_\beta - G_\alpha) + A\,\gamma + V\,\Delta G_{el} + V_{Ext}$

lattice ← **Monte Carlo** → displacements

While lattice MC gives time evolution (k-MC), it does so at the price of neglecting several terms in the driving force

Homogeneous Cu precipitation





Experimental determination of cluster composition in industrial ferritic steel

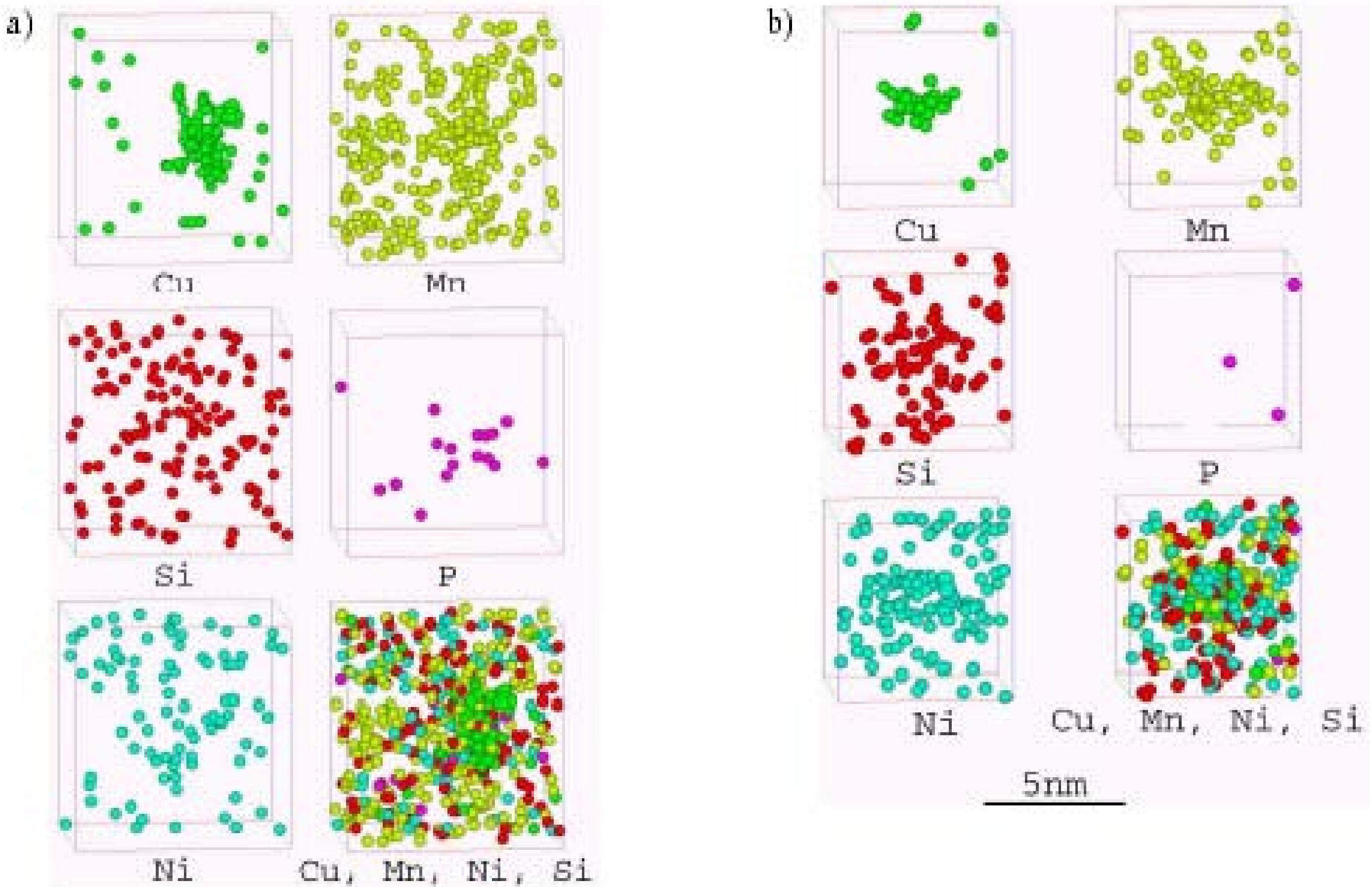
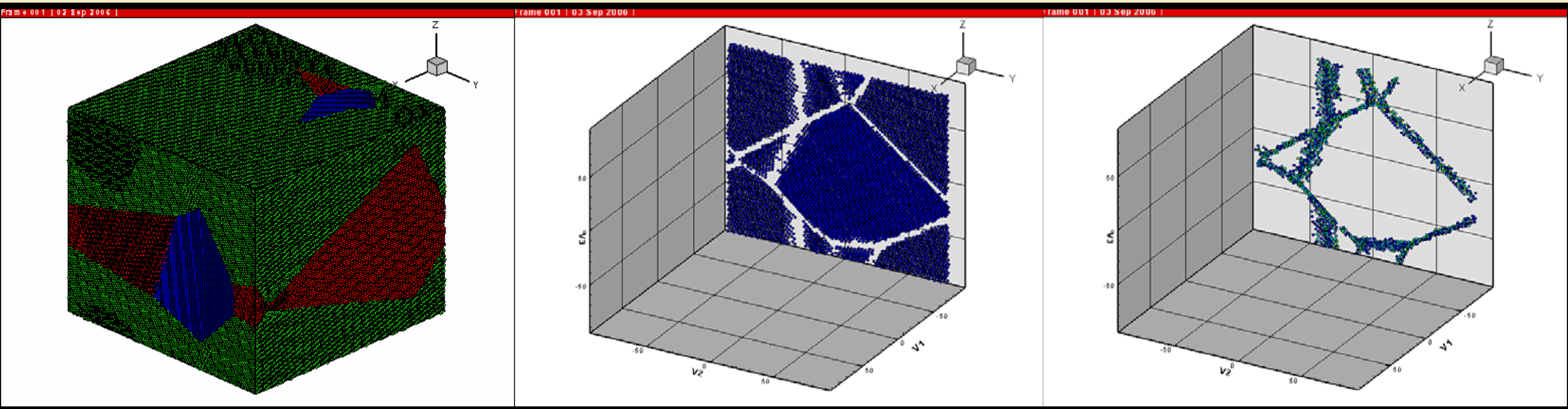


Figure 2. *Enlarged view of a) cluster 2 (extents of outline box 8x8x8nm^3) from 3DAP analysis of SH and b) cluster 8 from 3DAP analysis of WV012 (extents of outline box 6x6x6nm^3) showing distribution of Cu, Mn, Ni, Si and P.*

Strategy to show you several HETEROGENEOUS precipitation examples: a nanophase Fe sample

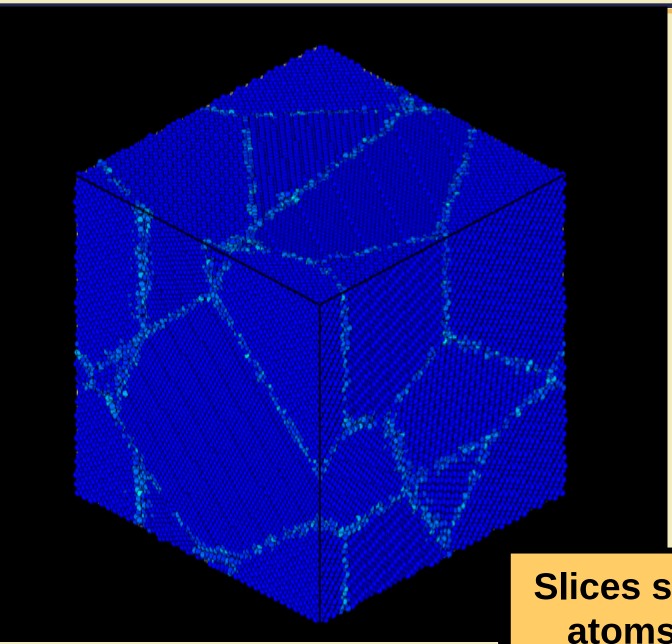


Nanophase sample 2 M atom, 15 grains	Slices showing perfect crystal bcc atoms	Slices showing grain boundary atoms

Heterogeneous precipitation in Fe-Cu

chemistry & materials science

CMS



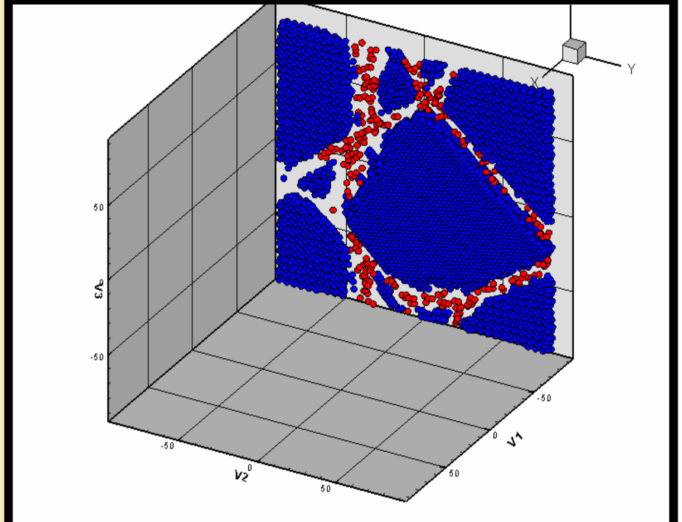
Bulk nanophase material

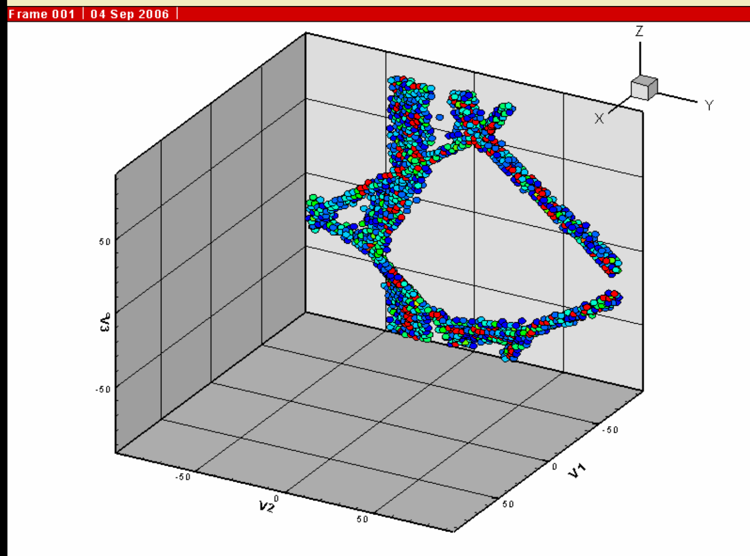
Cu has a strong tendency to precipitate

- at grain boundaries
- at junctions

3% Cu precipitation at grain boundaries in Fe

Slices showing perfect crystal bcc atoms in blue, Cu atoms in red

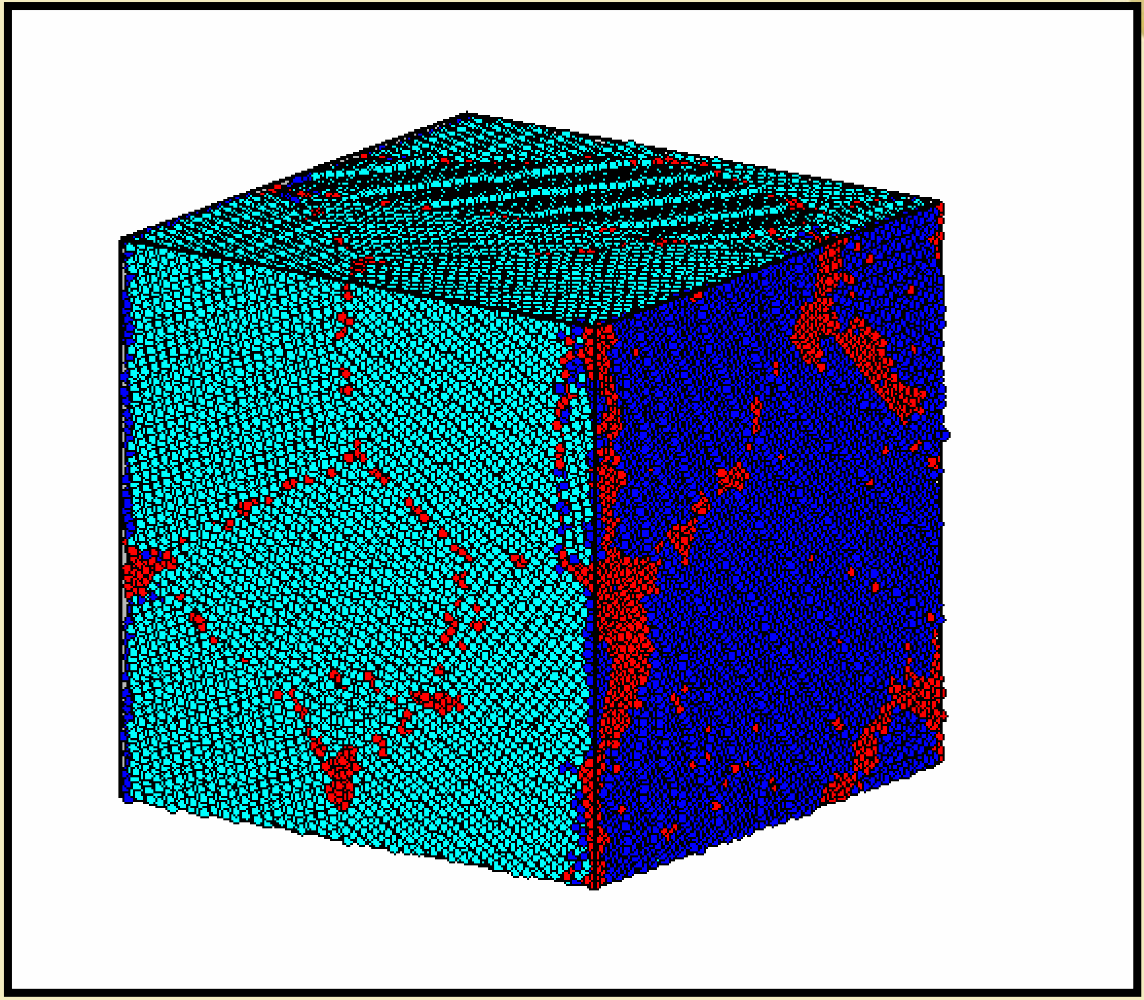




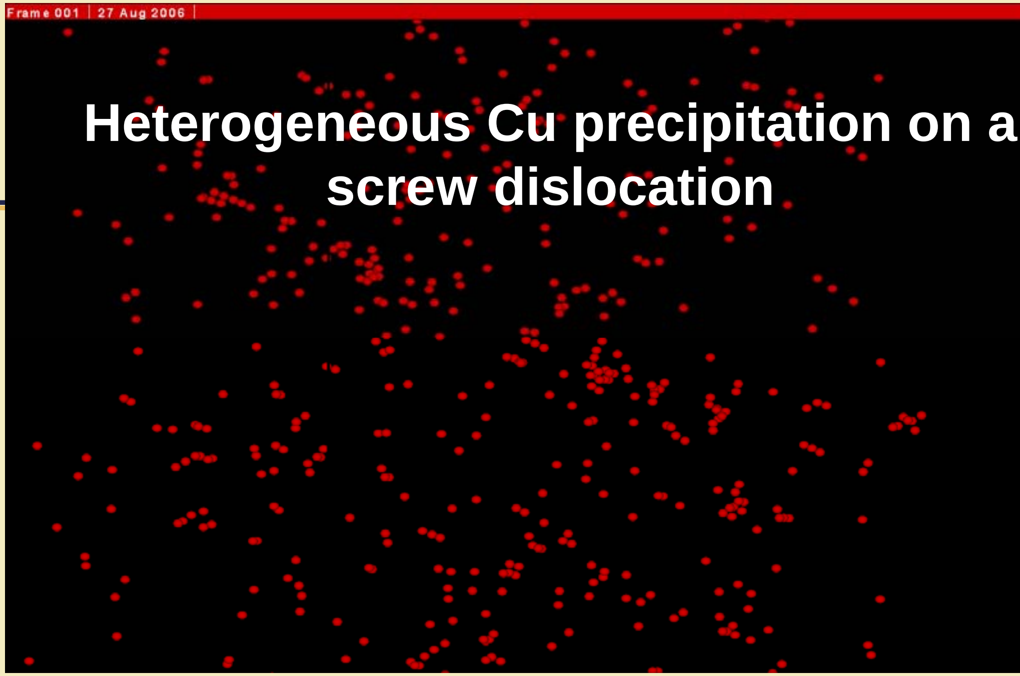
Heterogeneous Cu precipitation in the presence of a free surface

Free surface (dark blue) in a nanophase sample

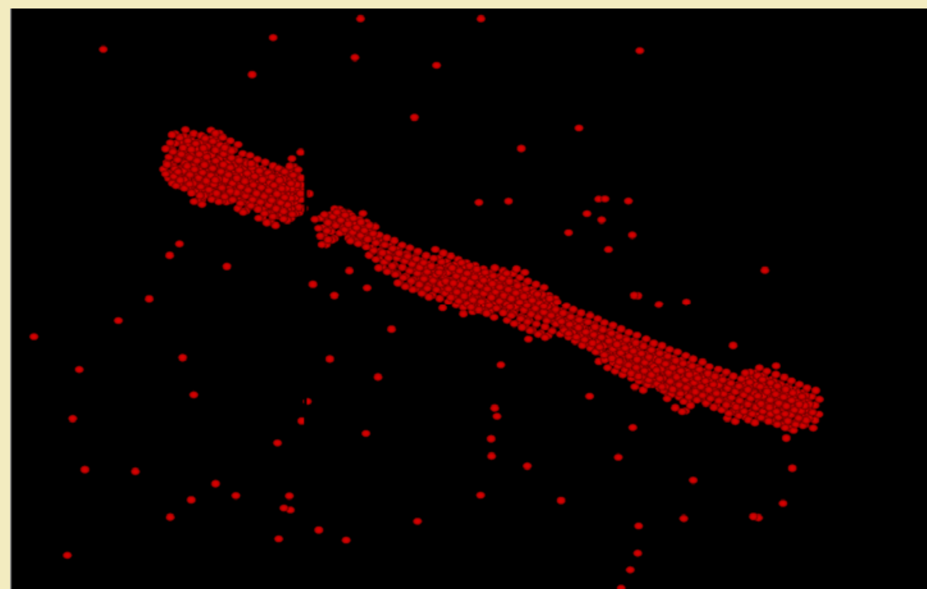
Cu goes preferentially to grain boundaries and triple-junctions that emerge at free surfaces



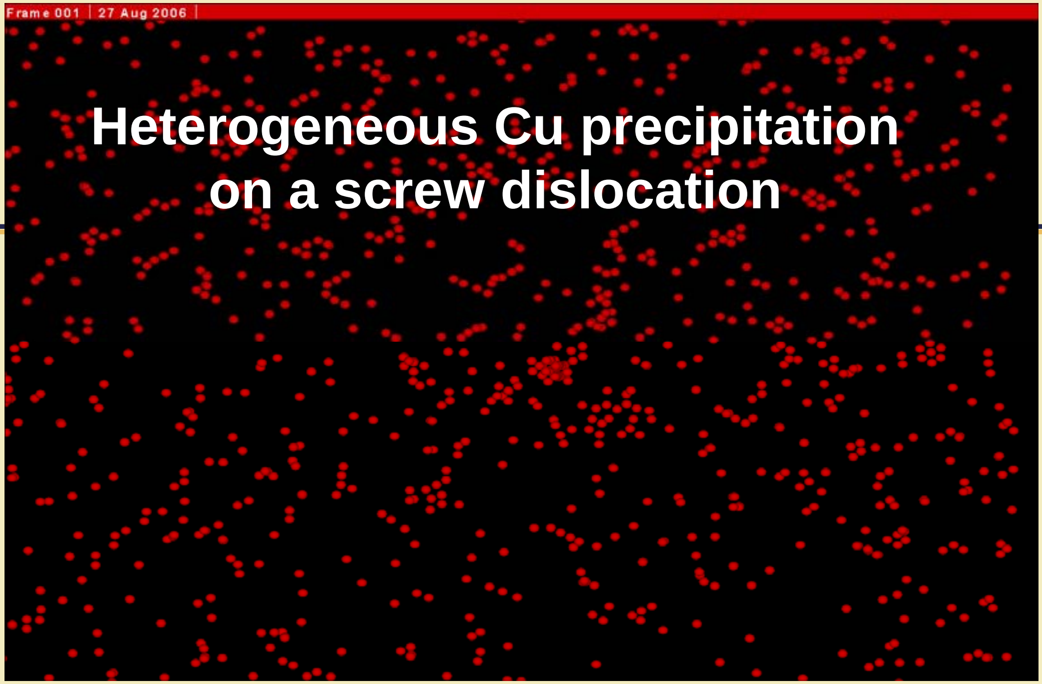
Heterogeneous Cu precipitation on a screw dislocation

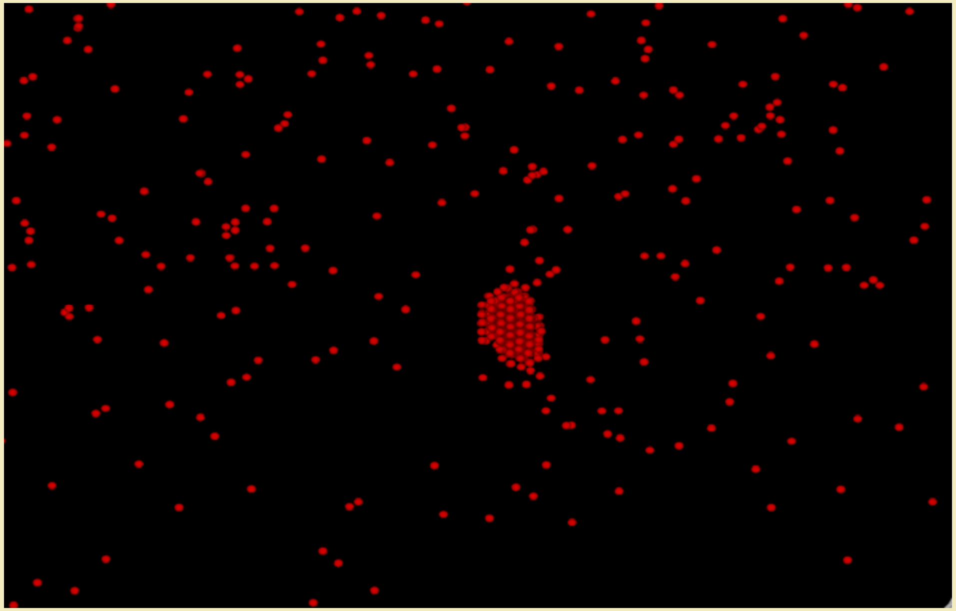


3% Cu precipitation at the core of a screw dislocation in Fe

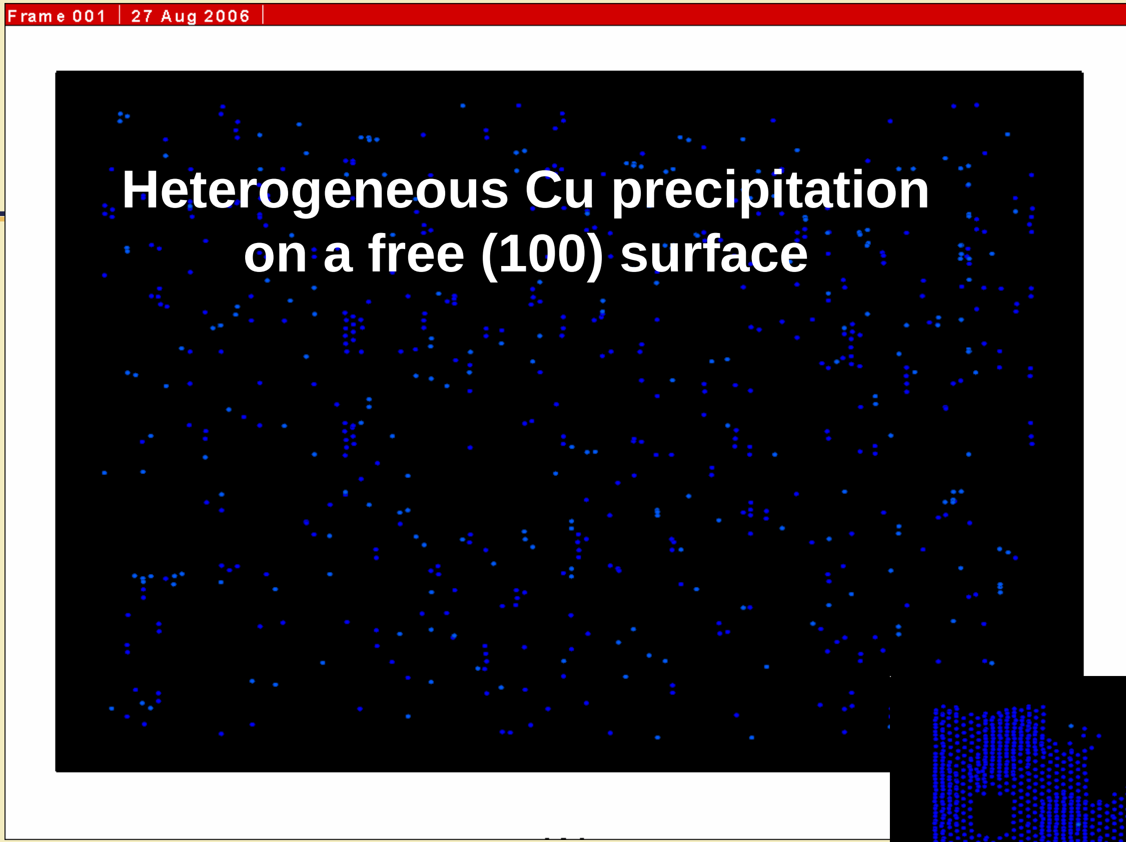


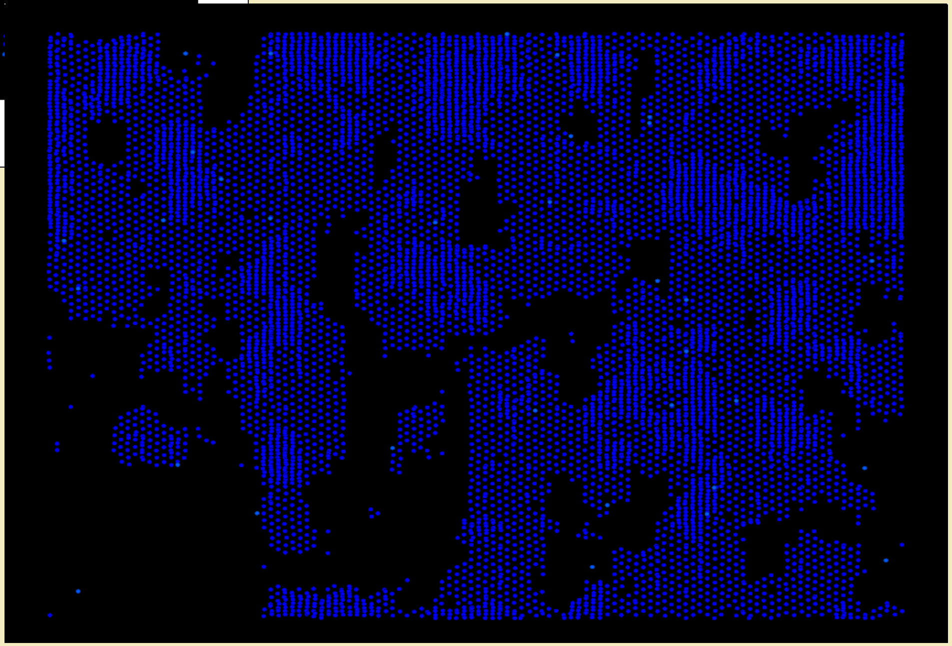
Heterogeneous Cu precipitation on a screw dislocation



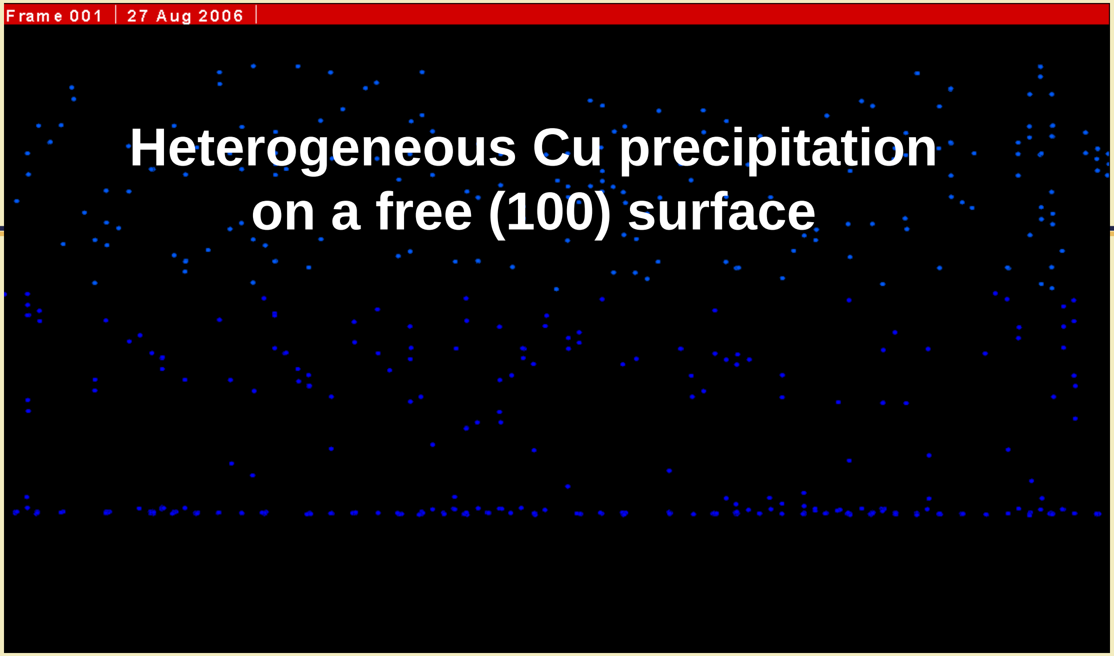


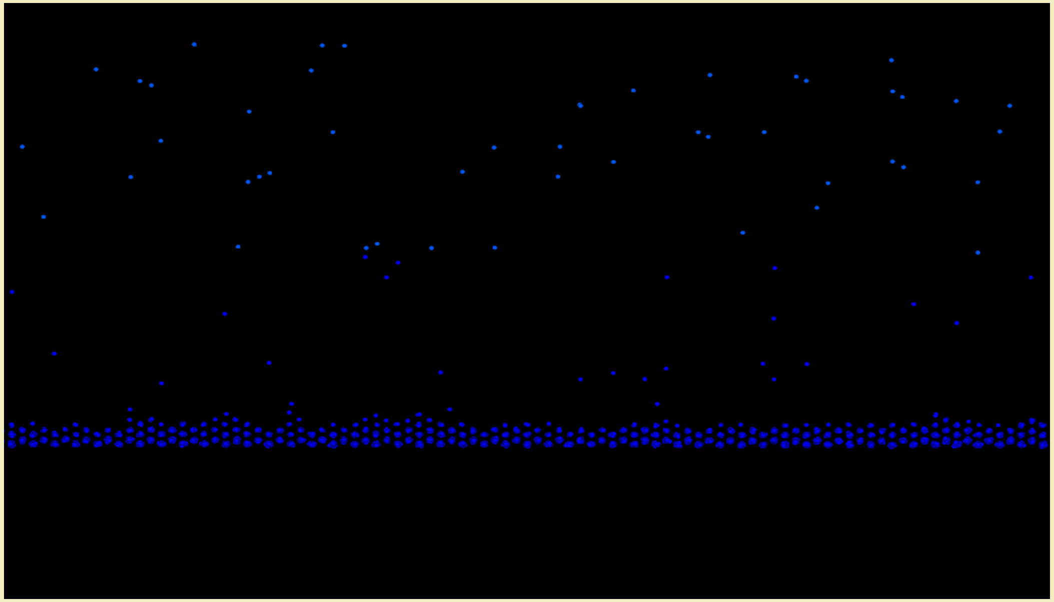
Heterogeneous Cu precipitation on a free (100) surface





Heterogeneous Cu precipitation on a free (100) surface





Conclusions:
New models and tools for computational modeling of alloys

Developments:

1 ✓ Formalism to design classic potentials for complex alloys

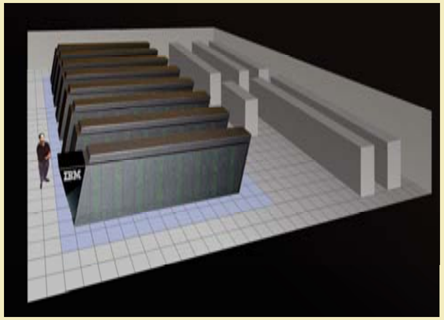
2 ✓ Thermodynamic package to evaluate free energies of alloys in any phase

3 ✓ Parallel Monte Carlo code with displacements, to predict equilibrium microstructures in alloys

Applications:

✓ An accurate description of the thermodynamics of the system allows us to study heterogeneous precipitation and obtain physically based microstructures

✓ We are studying the effect of precipitation on mechanical properties



Computational Materials Science