MatCASE

Materials Computation And Simulation Environment

(http://www.matcase.psu.edu)

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Supported by NSF under the grant number DMR-0205232

Project Personnel

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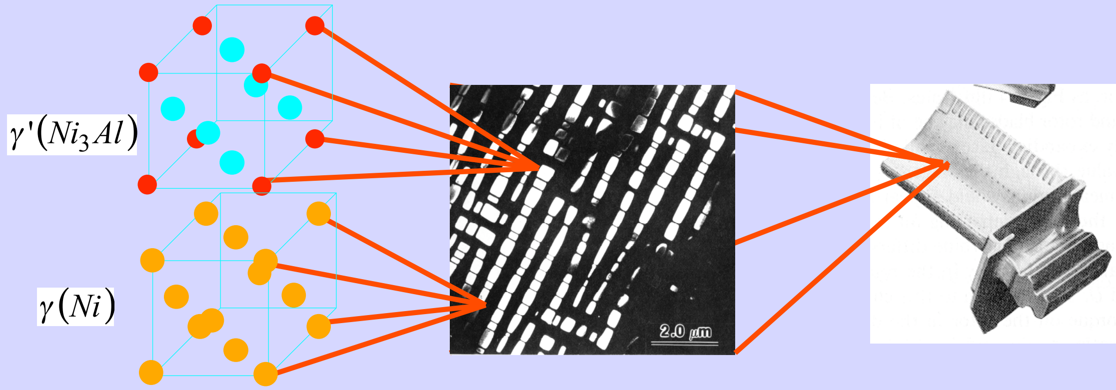
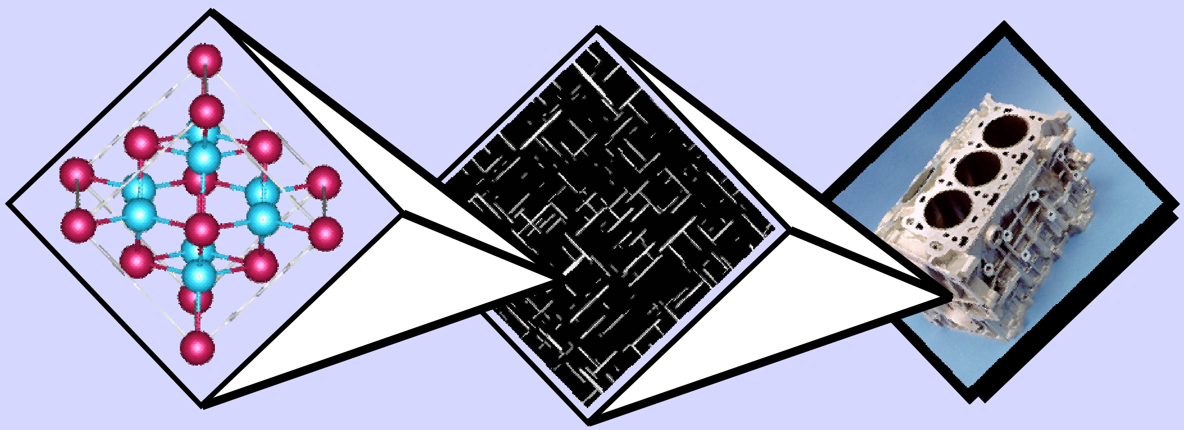
MatCASE Objective

Develop a set of integrated computational and information technology tools to predict the relationships among chemical, microstructural, and mechanical properties of multicomponent materials using the technologically important aluminum-based alloys as a model system.

Chemstry-Microstructure-Properties



Turbine Blade



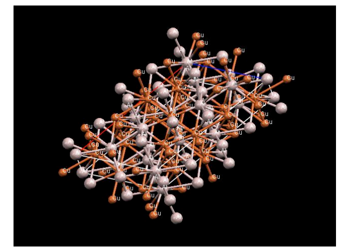
Atomic structure

microstructure

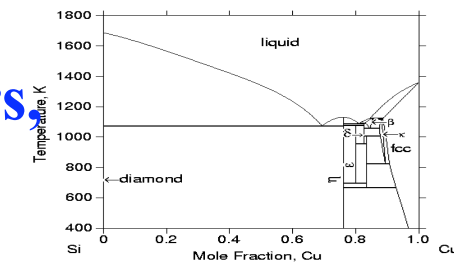
Engine Block

Four Major Computational Components

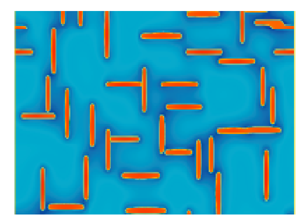
- First principles calculations of thermodynamic properties, lattice parameters, and kinetic data of unary, binary and ternary compounds



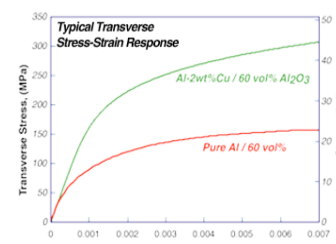
- CALPHAD data optimization of thermodynamic properties, lattice parameters, and kinetic data of multicomponent systems from first-principle calculations and experimental data



- Phase-field prediction of microstructures in 1-3 dimensions



- Finite element analysis of mechanical responses from the simulated microstructures



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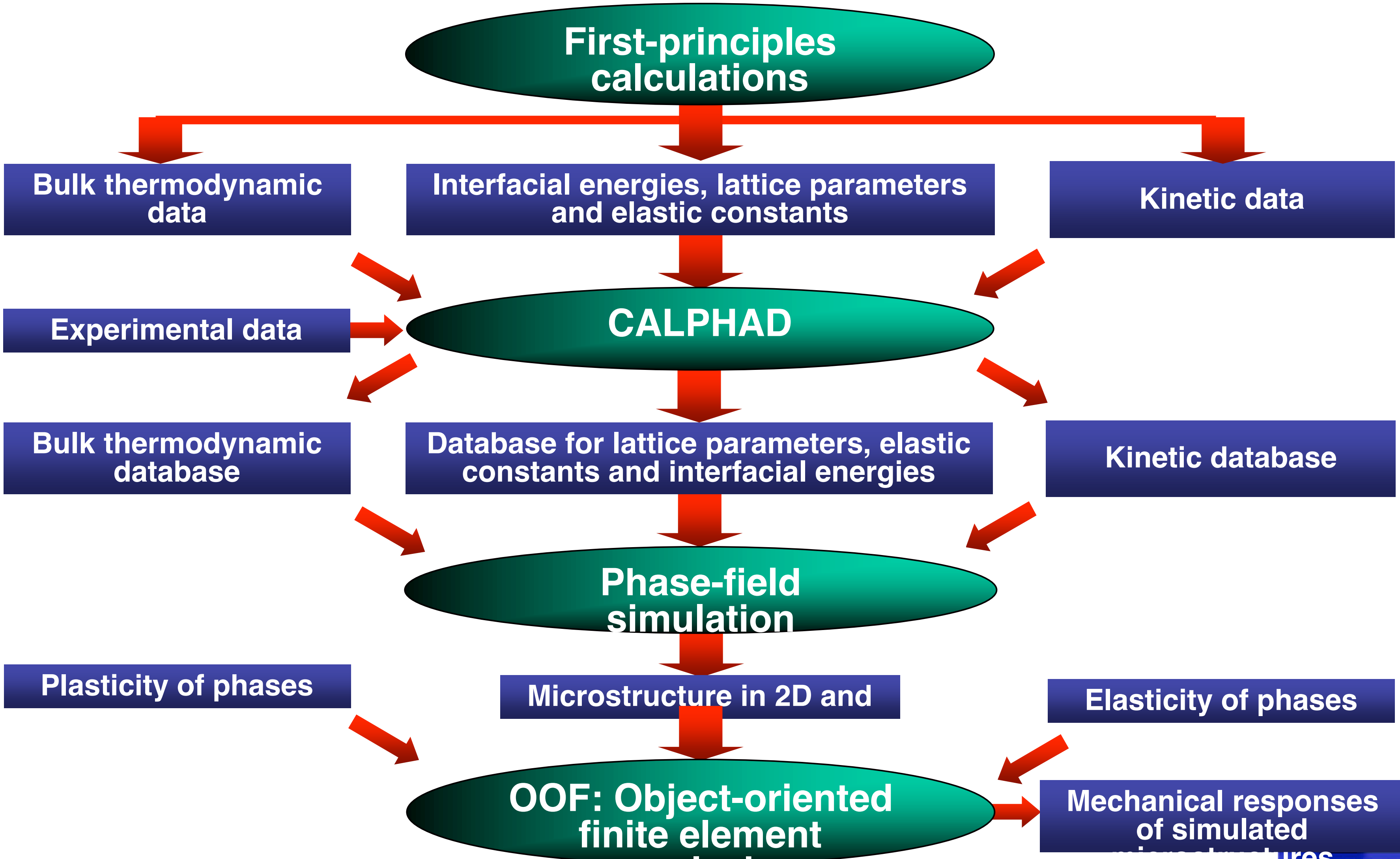
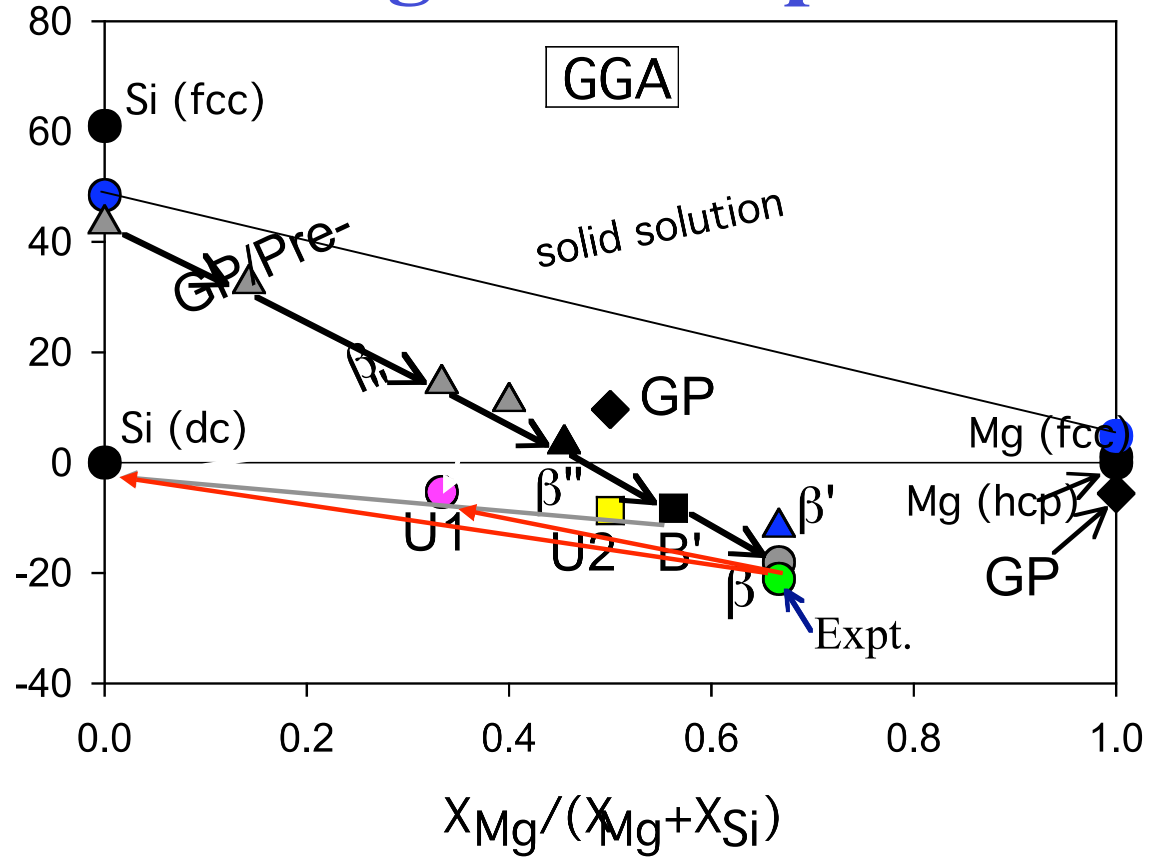
Integration of Four Computational Methodologies



First-Principles Calculations

- Energies of formation of metastable and stable compounds
- Interfacial energies of metastable and stable phases
- Vibrational entropies of metastable and stable phases
- Special Quasirandom Structures (SQS) for thermodynamic properties of solid solutions
- Mixed space cluster expansion / Kinetic Monte Carlo simulations of pre-precipitation cluster morphologies

First-Principles Energetics: Al-Mg-Si Precipitates



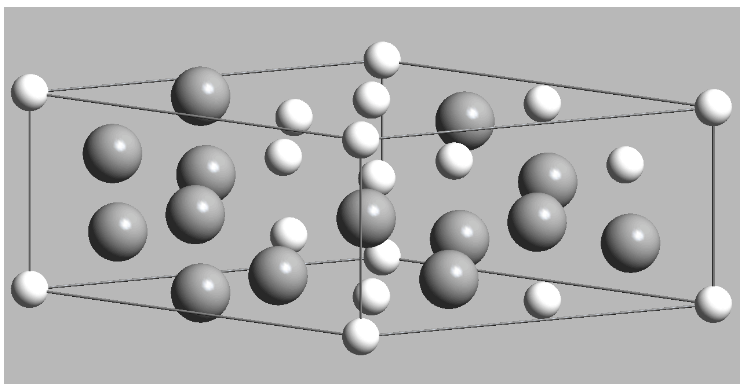
FP energetics correctly predicted the observed precipitation sequence:

ΔH(SS) > ΔH(GP/Pre-β′′) > ΔH(β′′) > ΔH(U1,U2,B′,β′) >ΔH(β)

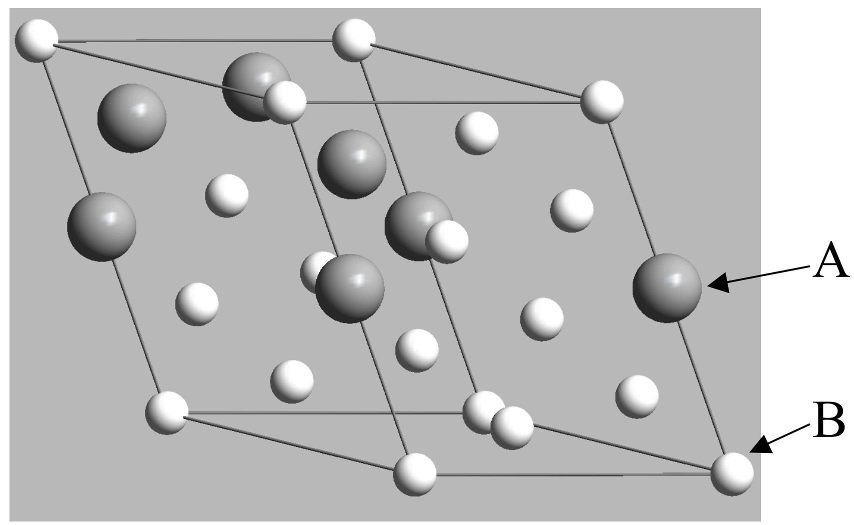
(C. Ravi and C. Wolverton 2004)

Special Quasirandom Structures (SQS's): A shortcut to obtaining alloy energetics

Three 16-atom SQS's were generated for random A_xB_{1-x} bcc alloys. They are small supercells which accurately mimic the most relevant correlation functions of the random alloys.



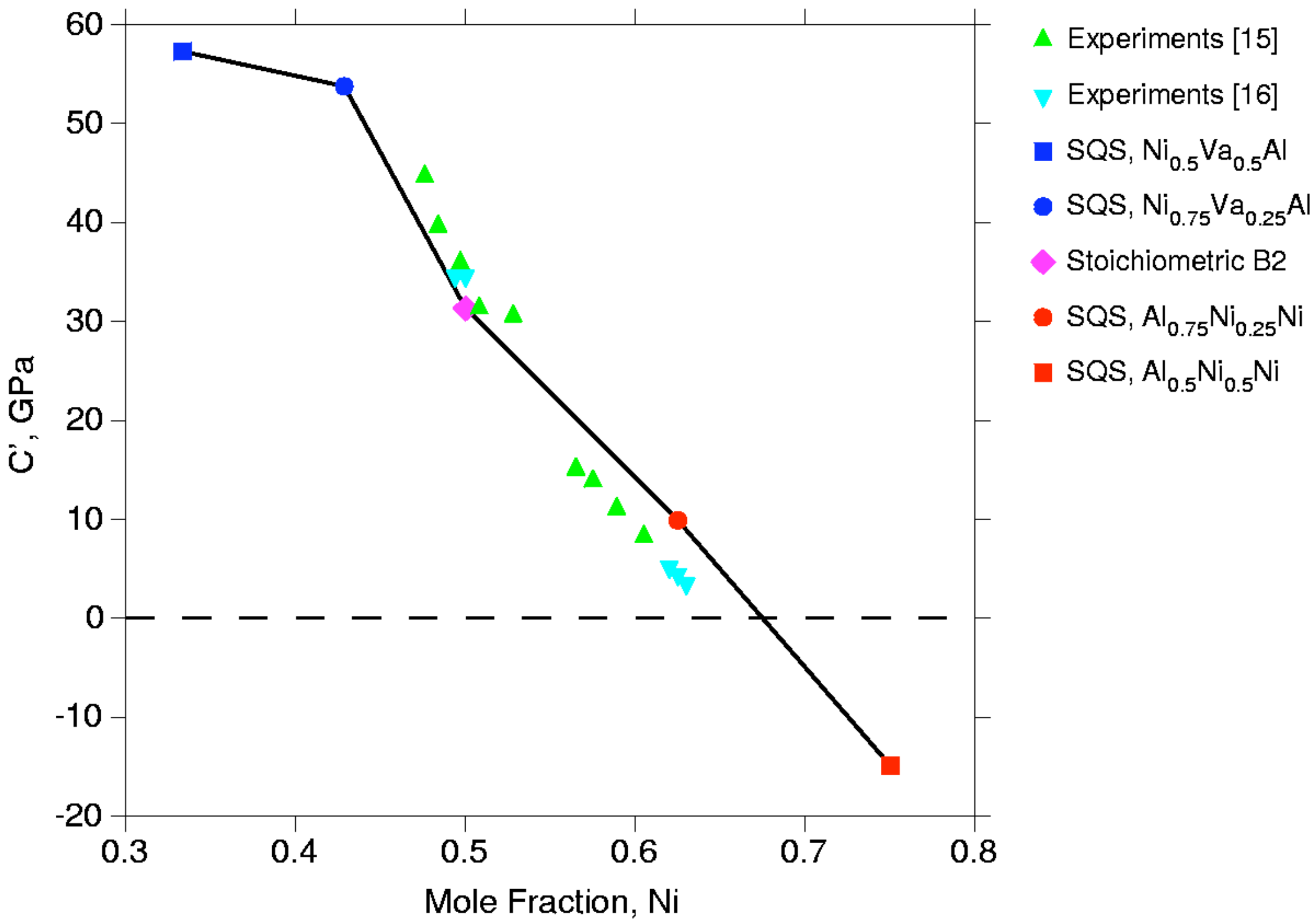
(a) 16-atom SQS for *x*=0.5



(b)16-atom SQS for *x*=0.75

(C. Jiang, C. Wolverton, J. Sofo, L. Q. Chen and Z. K. Liu, 2004)

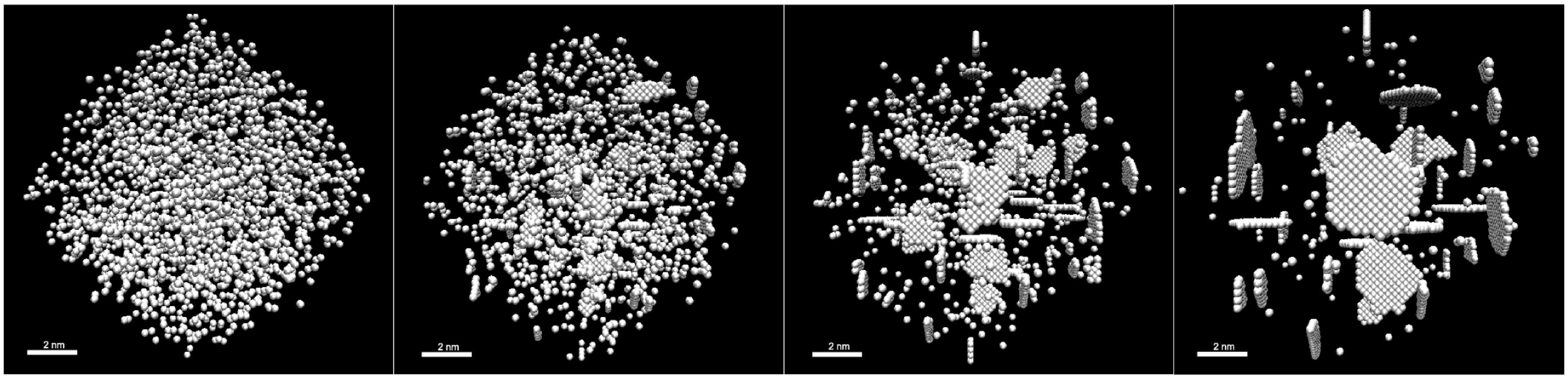
Prediction of B2 Stability



(C. Jiang, L. Q. Chen and Z.-K. Liu: 2004)

First-Principles Predicted GP Zone Nanostructure Evolution in Al-Cu

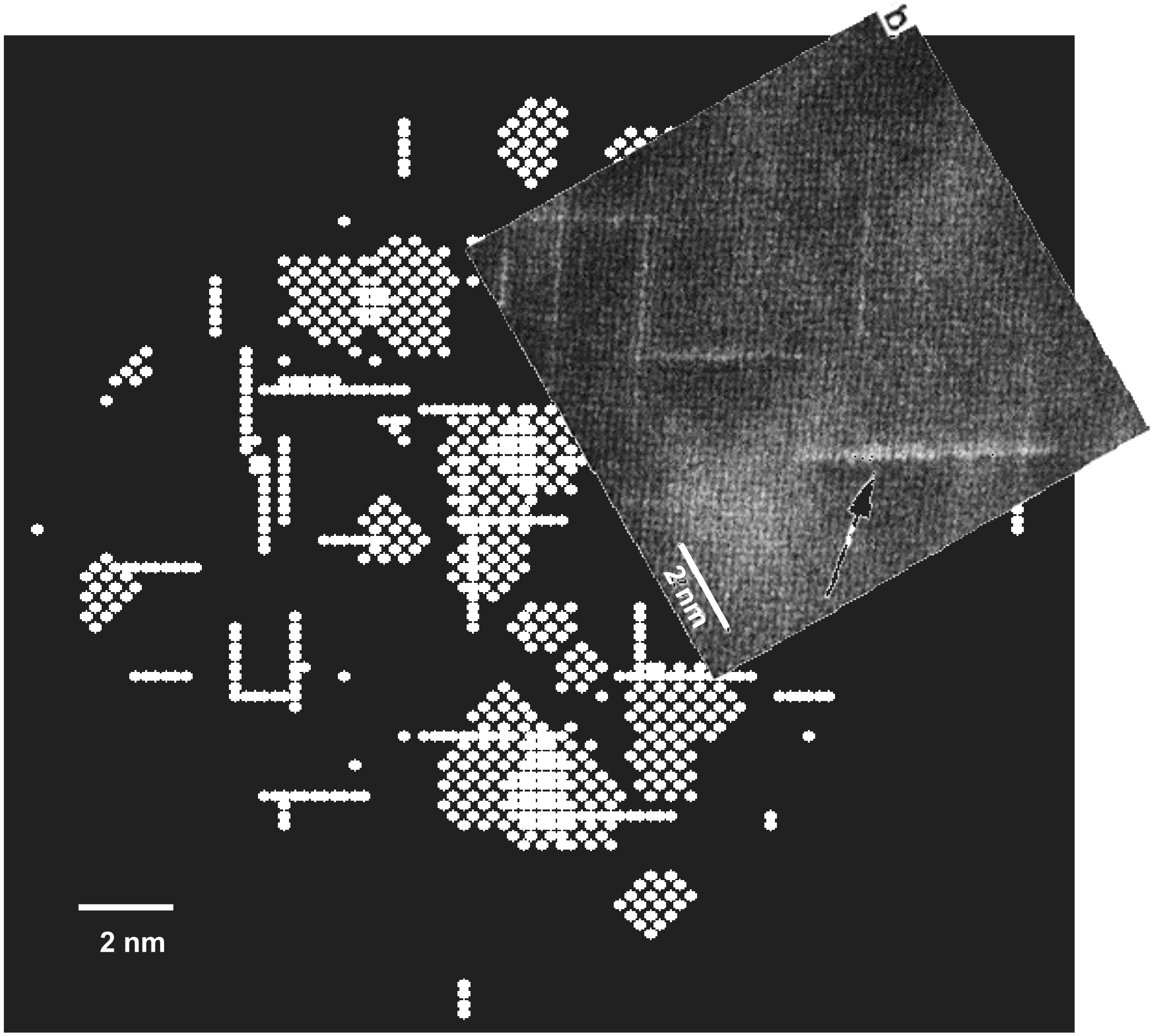
Solid Solution → **Nucleation and Growth** → **Coarsening**



t=0 $t=8*10^6$s $t=2.4*10^7$s $t=1.6*10^8$s

Mixed space cluster expansion / Kinetic Monte Carlo simulations
(J. Wang, C. Wolverton, Z.K. Liu, S. Muller, L. Q. Chen, 2004)

Comparison of Predicted and Observed GP Zone Nanostructure in Al-Cu



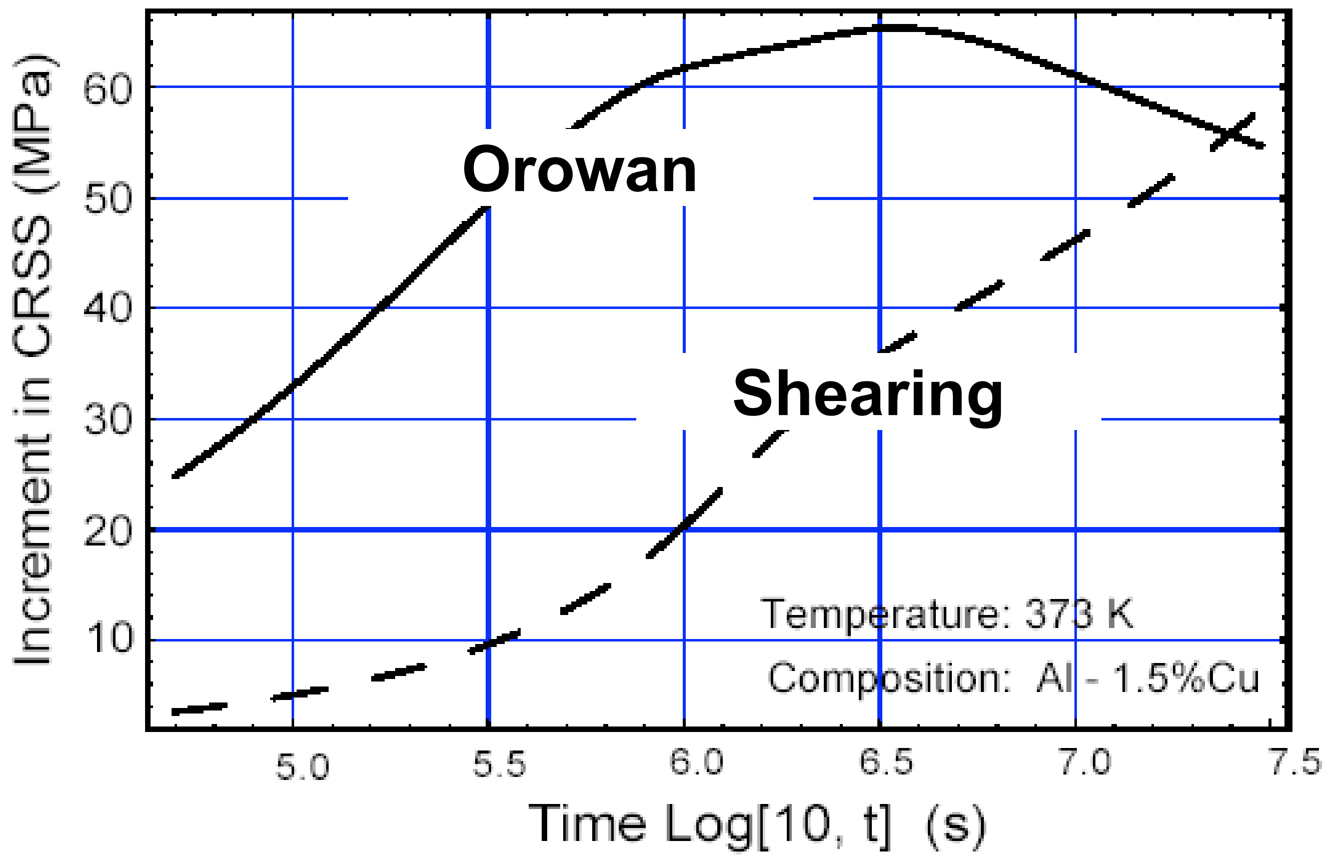
Simulation:
Al-1.0%Cu
T=373 K, t~1000 days

Experiment:
Al-1.4%Cu
T=300 K, t=100 days

HAADF
(high-angle annular detector dark-fiel d)
Konno et al., 2001

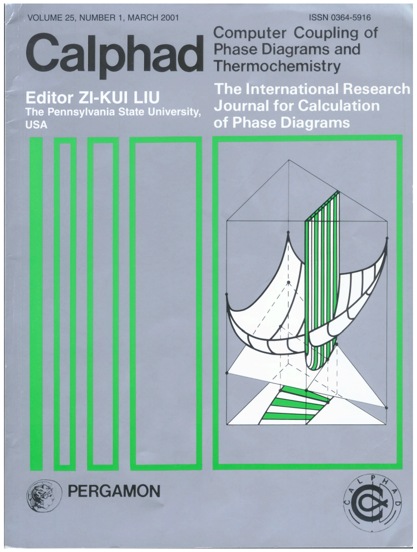
Mechanical Properties Prediction

— Shearing vs. Orowan Strengthening

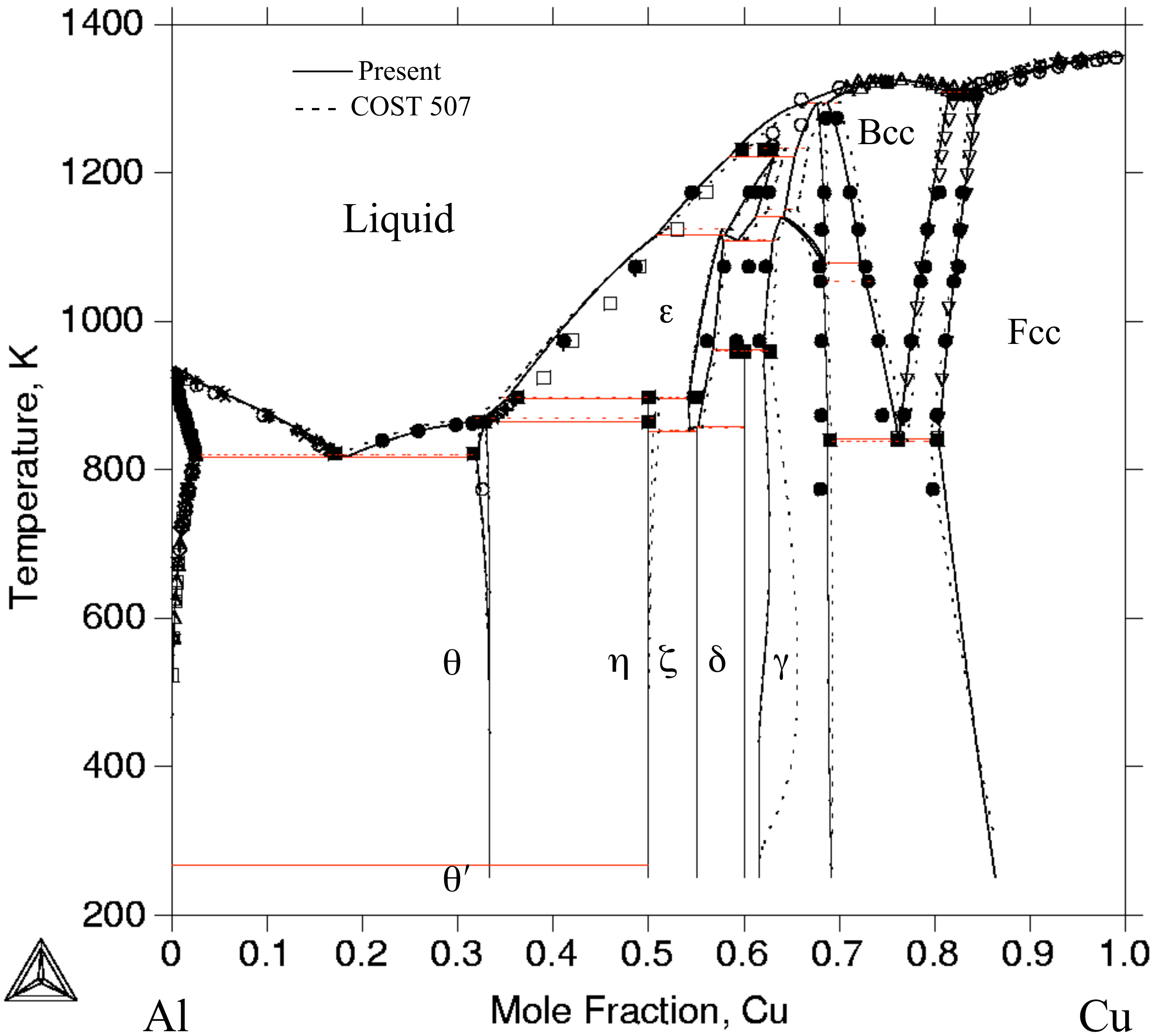


CALPHAD Modeling

- Gibbs energy functions of stable and metastable phases and phase diagrams
  - Input data: thermochemical and phase equilibrium data
- Lattice parameter
- Atomic mobility
- Automation in modeling

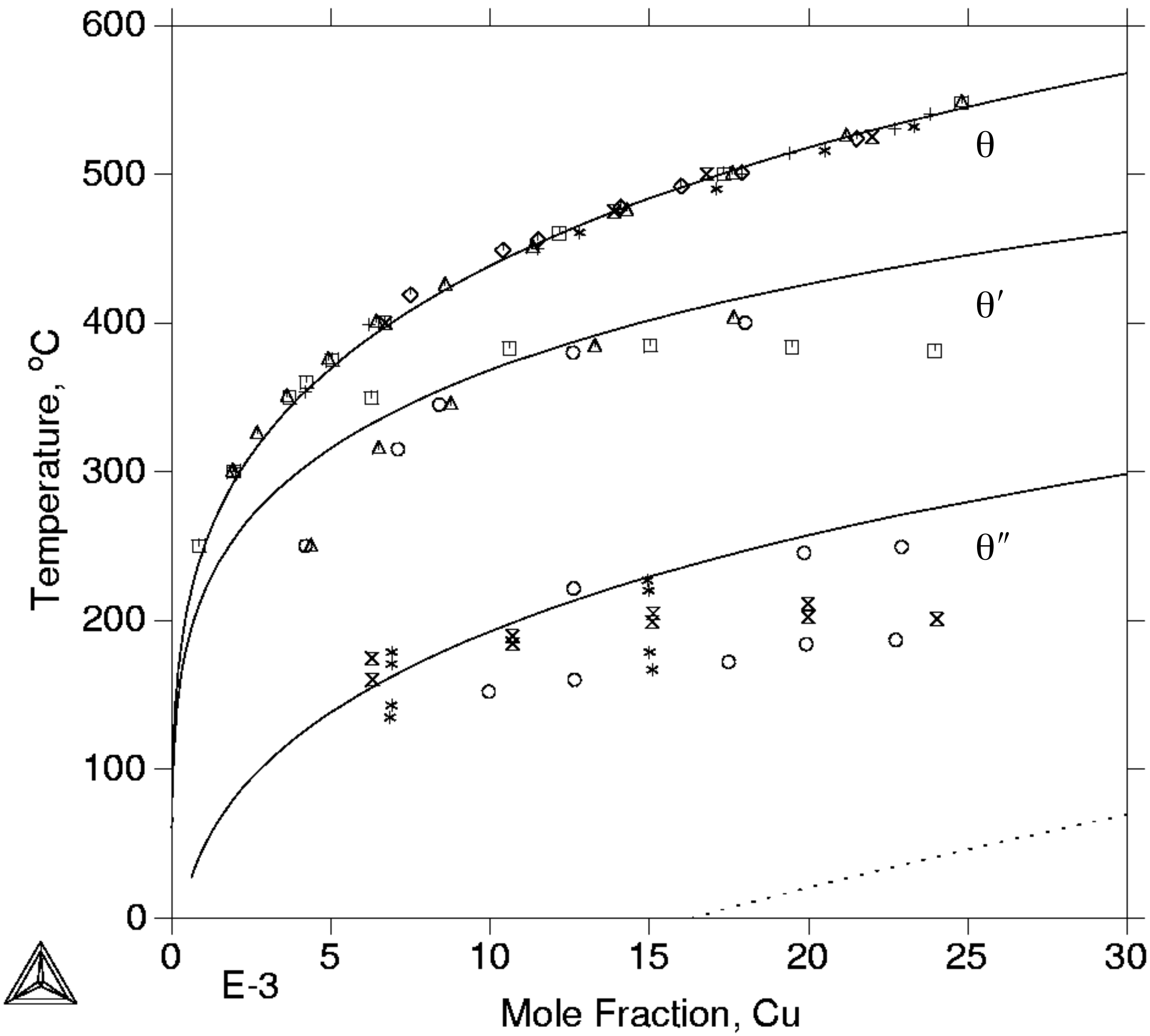


Al-Cu Phase Diagram

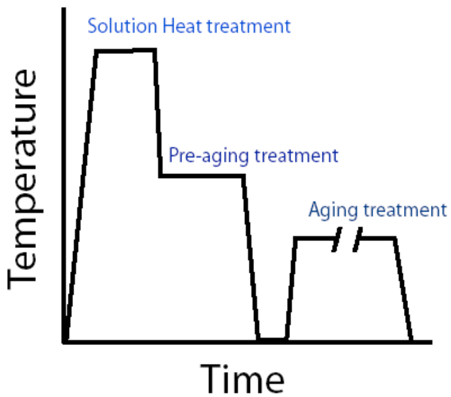


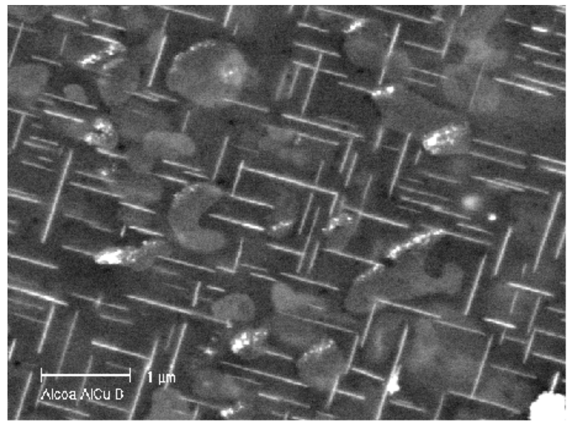
(C.Jiang et al 2004)

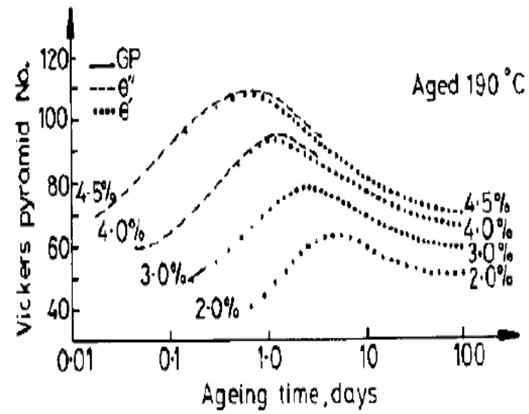
Solvus of Metastable Phases

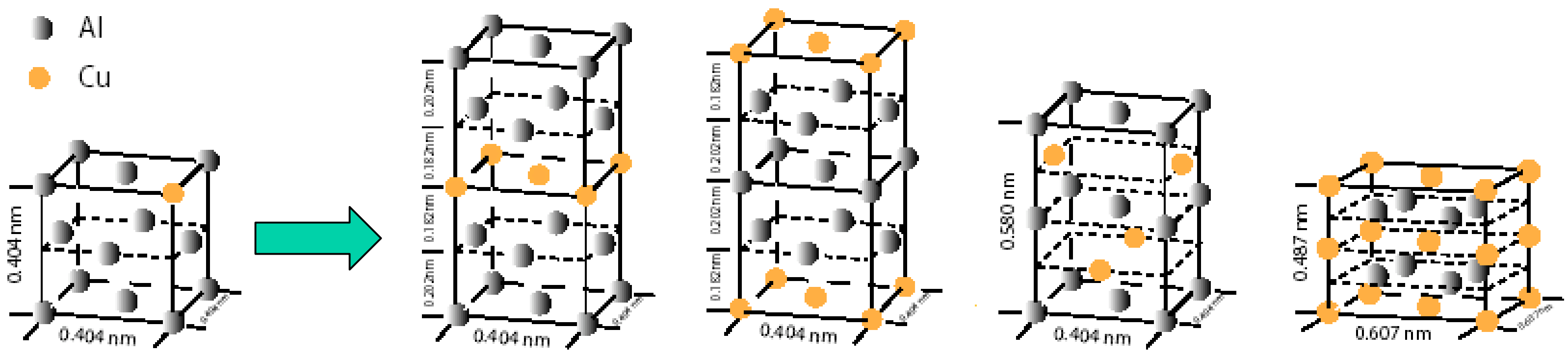


Phase-field Simulations of Precipitation in Al-Cu Alloys





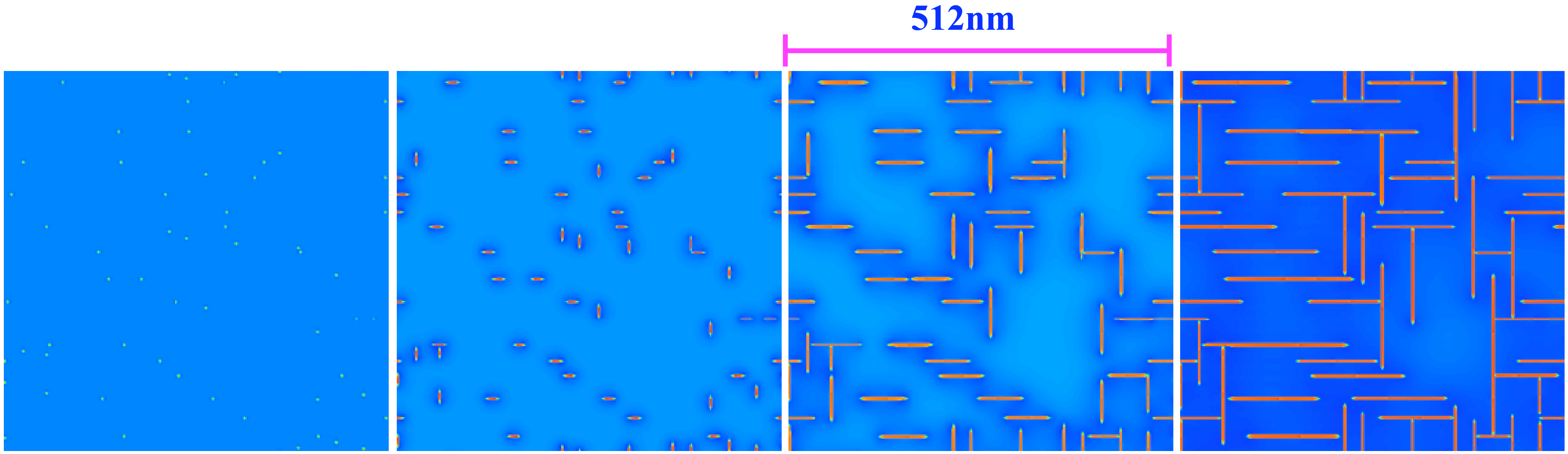




α GP θ'' θ' θ

θ´ Precipitation

Al-1.8at%Cu at 500K with nucleation at dislocations

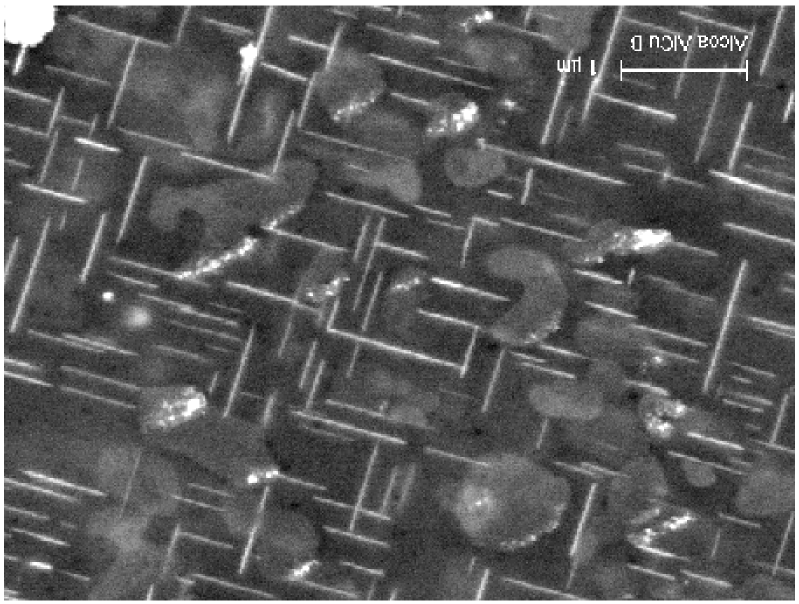


t=3mins | t=8.8mins | t=41mins | t=85mins

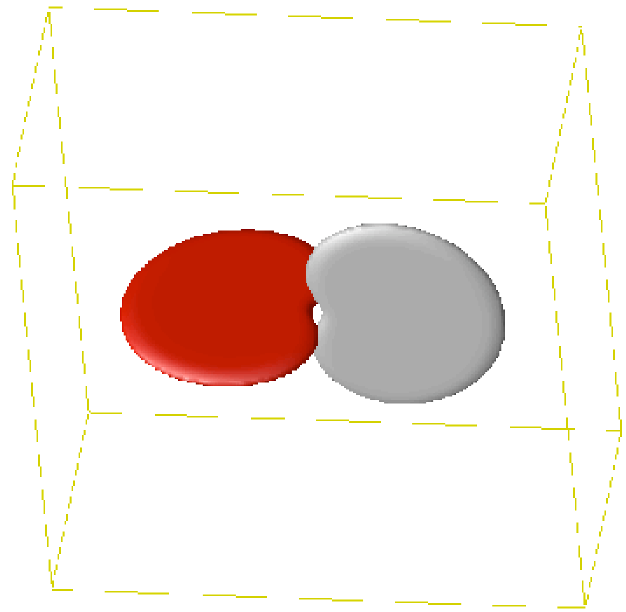
Time

(S. Y. Hu et al 2004)

Comparison of θ' Morphologies in 3D

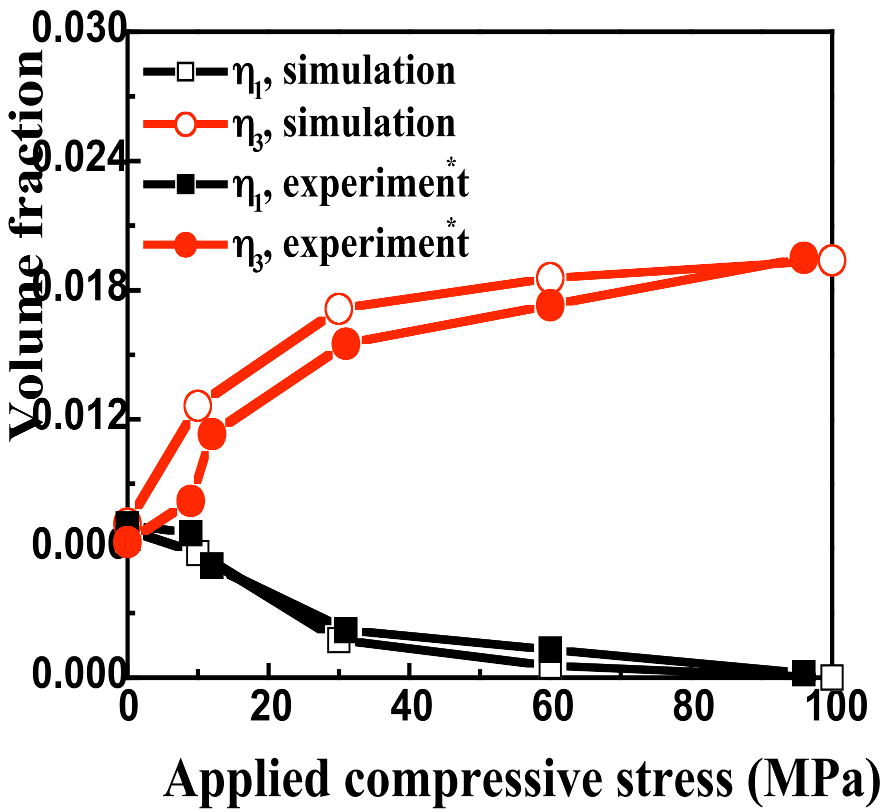


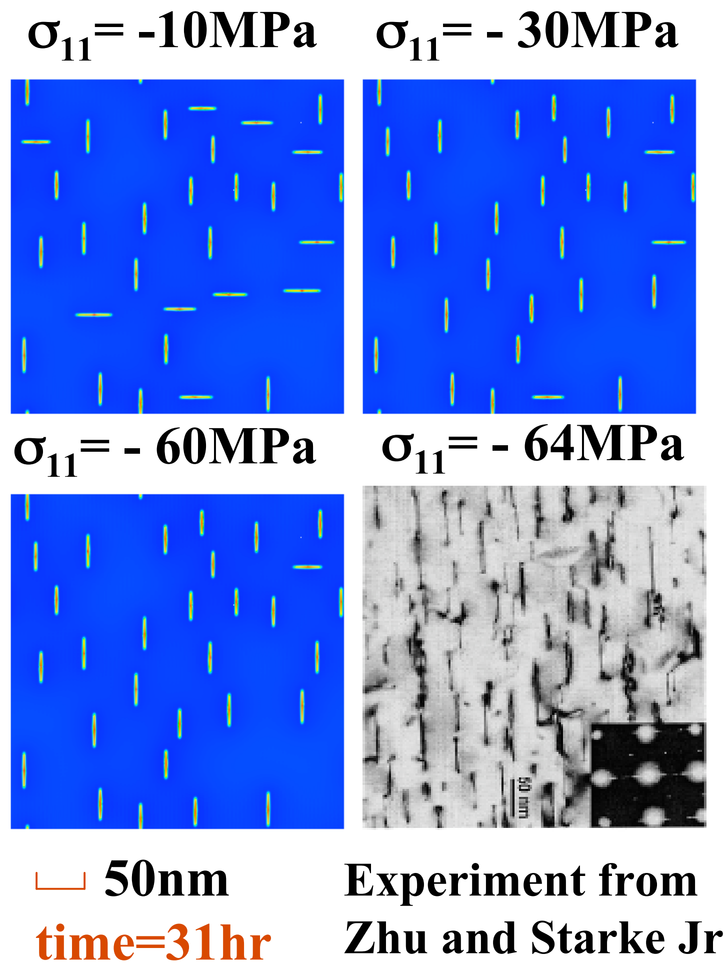
Experiment from H. Weiland



Simulation

Comparison of simulation and experiment of stress aging at T=453K

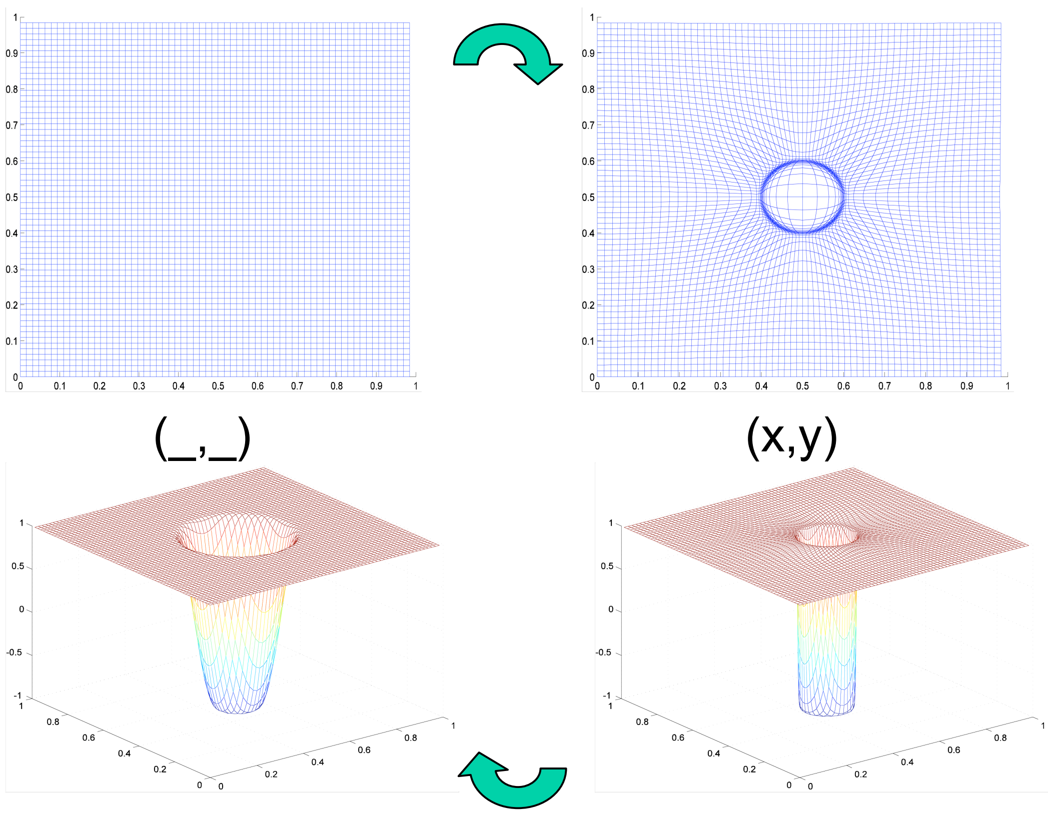




Experiment from Zhu and Starke Jr

(Seol et al 2004)

Phase-Field Simulation on Adaptive Grids by Moving Mesh PDEs



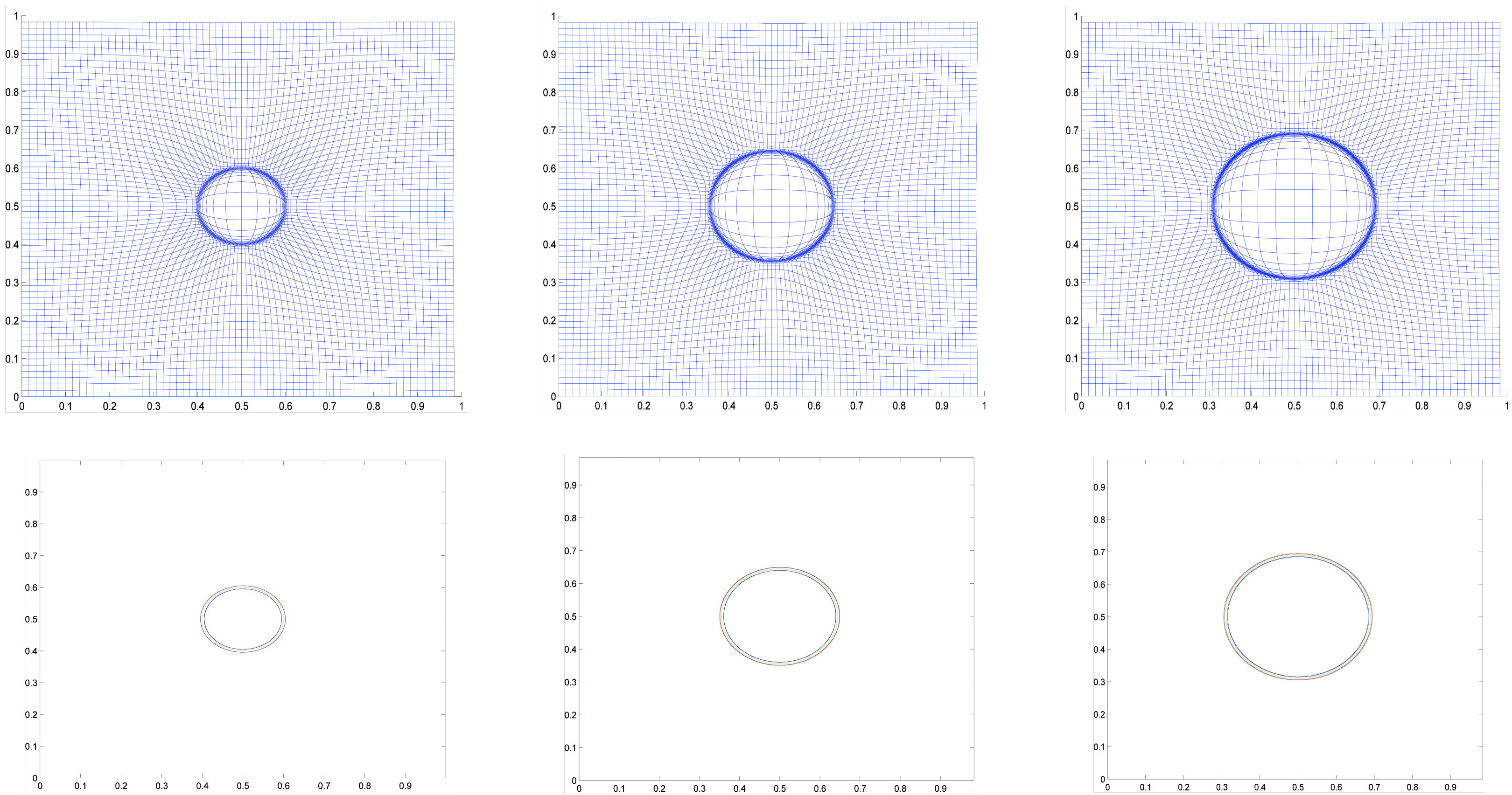
Phase variable on computational domain

Phase variable on physical domain

Construct a mapping from the computational domain to the physical domain (_,_)_(x,y) so that the solution in the computational space is "better behaved".

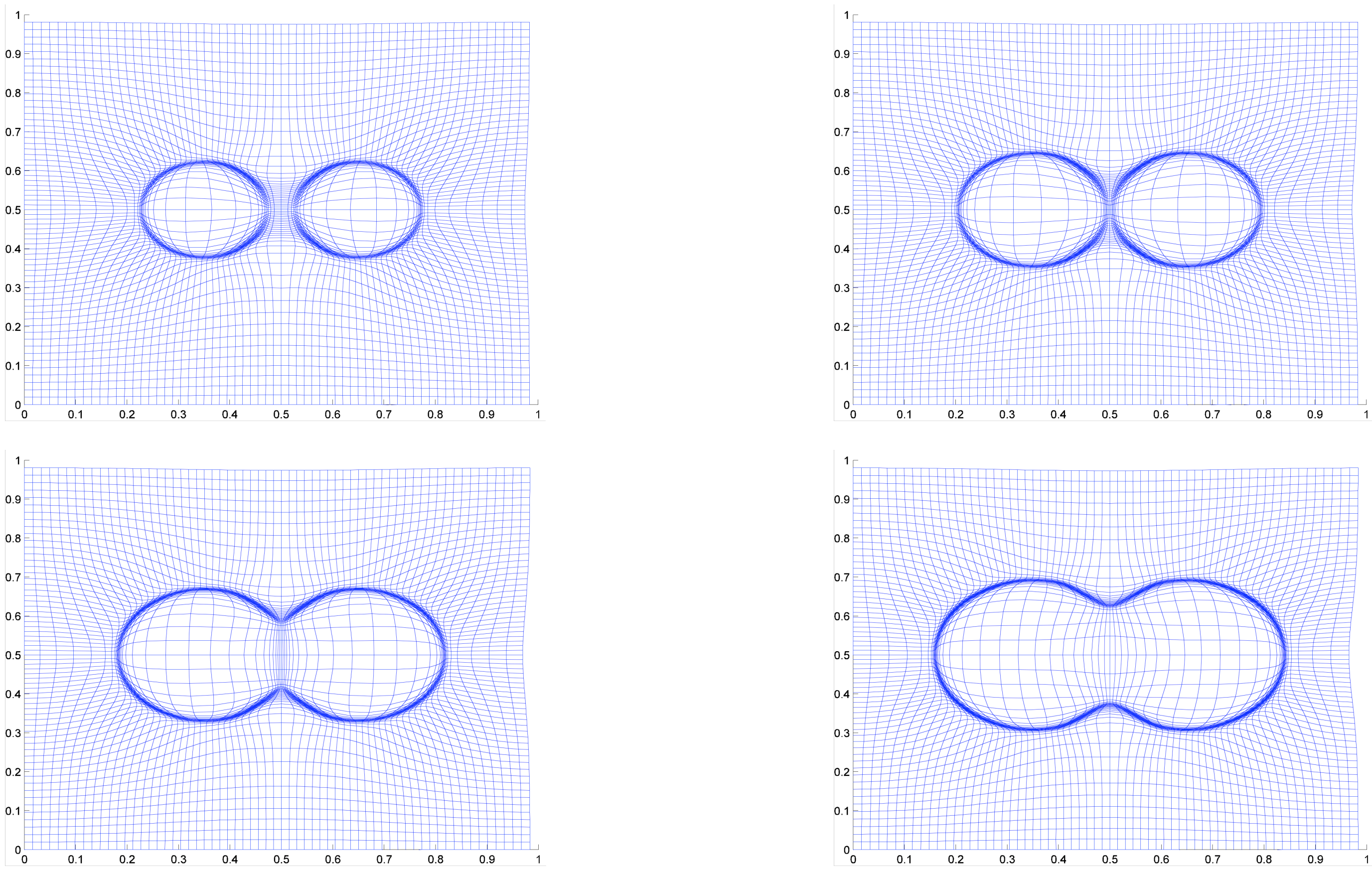
(Y. Peng et al 2004)

A Simple Test Run: Single Particle Growth



Comparison of interfacial contour plots by 64*64 adaptive grid (CPU time: 1 min) **and those by 512*512 regular grid** (CPU time: 6 mins).

Handling Topological Changes



Attractive Features of the Moving Mesh Approach

- Keeps the applicability of the Fourier-Spectral method to efficient numerical solution of the phase-field equations.
- Mesh gradually adapts to the phase variable. Thus particularly suitable for moving interface problems.
- MMPDE can also be solved using semi-implicit Fourier-spectral scheme.
- Monitor function smoothing via convolution can be performed in Fourier-space as well.

Information Technology Tool Development

- Web-portal for material scientists to explore macrostructural properties of multicomponent alloys

- We are developing:
  - information base of material properties obtained from experiment or simulation, includes lattice structures, enthalpies, specific heat, potential energies etc.
  - Rule database of properties of the tools for the main steps, their underlying models, limitations, verifiable range of results, error states

- We automate design space exploration by composing knowledge bases with scalable simulation tools for the four main steps
- Back-end of e-laboratory supports wide-area grid computing where local sites can have high-end multiprocessors and clusters

User View

- Users (clients) connect to initiate materials design via web-portal
- Web-portal creates a service to the user and executes remote tasks
- Remote tasks are managed by Globus-enabled services
  - Automatically specifies exact set of simulations needed to compute missing data for a given design
- Our model reuses information in materials databases as much as possible

Design Challenges

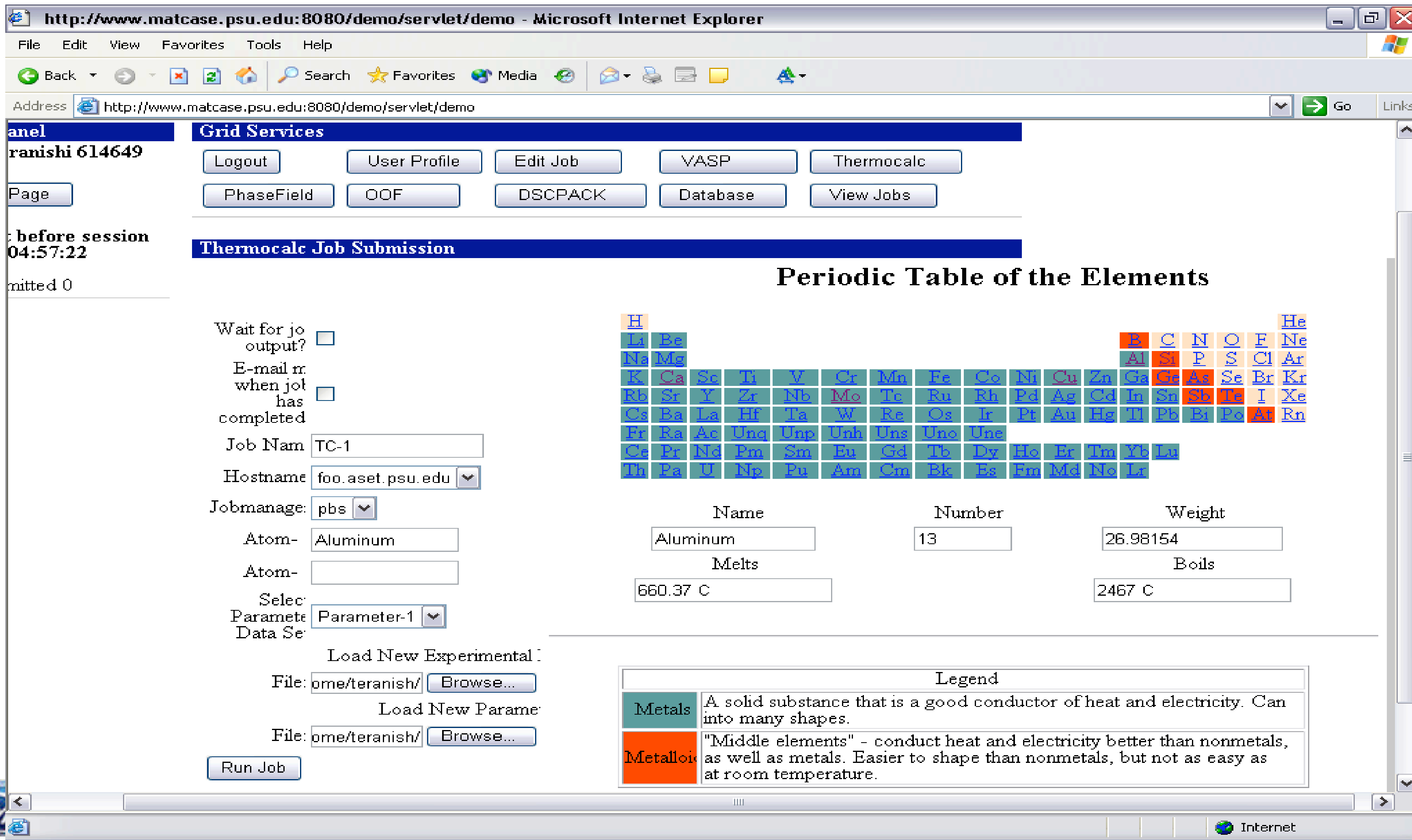
- Identifying data necessary for each of the four main steps
- Providing a default form of inputs for each tool (more than one for a step)
- Translating results between tools for successive steps
- Managing workflow of tasks from many clients
- Automatically analyzing intermediate results to provide meaningful simulations (i.e. avoid cascading bad simulation results, detecting failures to converge, etc.)

Three Part Services-Based System

- A reconfigurable web portal system with 3 main components
  - Interaction handler
    - Gets input from clients and provides intermediate/final results
  - Analyzer
    - Creates instances of interaction and simulation handlers
    - Manage "rules" for meaningful composition
    - Bridge between interaction handler and simulation handler for each client
  - Simulation handler
    - Executes remote tasks using Globus grid-services
    - Creates instances of local "services" to process input/output between steps
    - Transfers input/output for client between the server and remote computers

Web-Portal for Design Space Exploration with Distributed HPC

Sample Screenshot



MATCASE and beyond…

- **Forward mode: What are the macro-structural properties given material specification? (current)**

- **Reverse mode : What are the materials with the desired macro-structural properties? (future)**

  – **Extensions to knowledge base, automated similarity detection, search through simulation, compact feature representation,…**