MedeA UNCLE

Explore Phase Stability, Bridge the Length Scales

At-a-Glance

MedeA ®[1] *UNCLE* (UNiversal CLuster Expansion)[2,3] expands access to materials and properties at the meso and micro scale, while maintaining the predictive power and accuracy of *ab-initio* Density Functional Theory (DFT) methods. Explore order-disorder phenomena and phase segregation processes as a function of temperature and composition.

Key Benefits

- Models systems containing millions of atoms with DFT accuracy
- User friendly setup within *MedeA Environment*
- Workflow based automation of cluster expansion refinement
- Efficient handling of hundreds of input structures
- Intuitive graphical analysis and visualization
- Split and restart complex calculations
- Extend and expand existing Cluster Expansions

Cluster Expansion with *MedeA UNCLE*

MedeA UNCLE lets you determine stable multi-component crystal structures and rank metastable structures by enthalpy of formation, while maintaining DFT accuracy. VASP *ab-initio* calculations are performed on automatically chosen sets of small models to obtain effective interaction parameters. Use these in a Monte Carlo simulation to capture the configurational complexity of real materials at different temperatures.

> *'On the one hand, cluster expansions are used to treat systems ranging from a few up to a million atoms without giving up the accuracy of modern DFT calculations. On the other hand, Monte Carlo simulations permit us to study finite-temperature properties such as short range order phenomena or mixing enthalpies.'*
>
> Stefan Müller (introduction of [3])

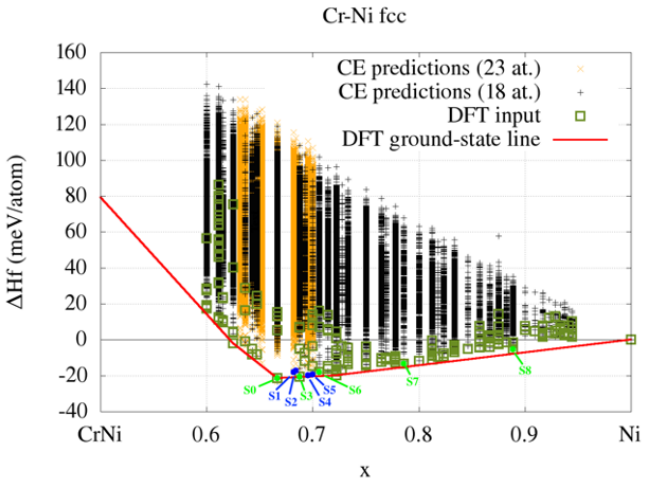

Fig. 1: Ground state diagram (convex hull) for the Cr-Ni system

Tight integration with *MedeA*'s job control guarantees ease of use, stability, and fault tolerance. Monitor progress of these fully automated calculations, and use graphical tools to readily visualize results.

Properties from *MedeA UNCLE*

- Ground state diagram (convex hull)
- Structures of stable phases
- Vacancy concentrations
- Miscibility

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

[2] D Lerch, O Wieckhorst, G L W Hart, R W Forcade, and S Müller, *Modelling and Simulation in Materials Science and Engineering* **17**, no. 5 (June 4, 2009): 055003.

[3] Stefan Müller, "Bulk and Surface Ordering Phenomena in Binary Metal Alloys", *Journal of Physics: Condensed Matter* **15**, no. 34 (August 15, 2003): R1429–R1500.

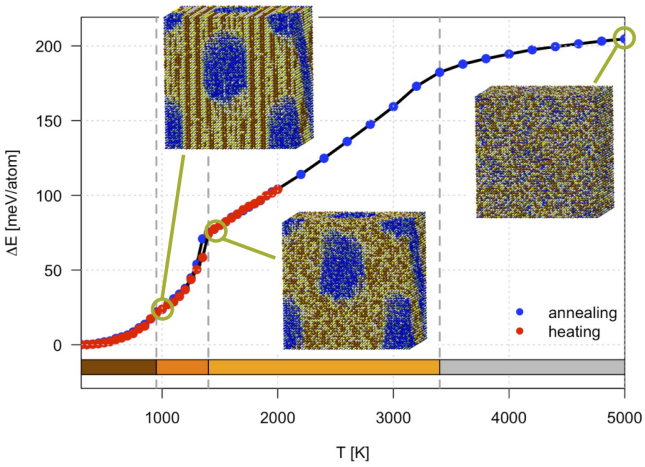

Fig. 2: Monte Carlo temperature profile (heating and cooling curves) and simulation cells for a 5 component high-entropy alloy

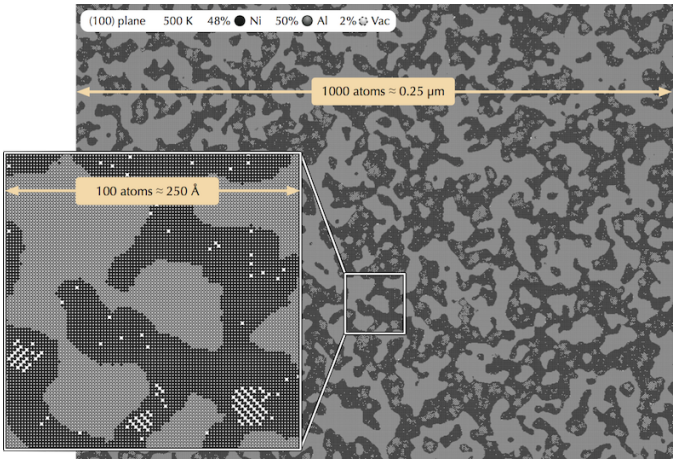

Fig. 3: NiAl alloy: (100) cut through a 1000 x 1000 x 1000 simulation cell superlattice with 2% constitutional vacancies at T = 500K.

- Random mixing energy
- Phase stability as a function of temperature and concentration
- Solubility
- Order-disorder transition temperature
- Microstructure
- Short range order parameter
- Surface segregation
- Surface coverage of adsorbents

Computational Characteristics

- Use Genetic Algorithm or Compressive Sensing
- Full integration with *MedeA VASP* and other modules
- High-throughput using the *MedeA JobServer*

Required Modules

- *MedeA Environment*
- *MedeA VASP*

Find Out More

Learn more about *MedeA UNCLE* applications and examples by watching the webinar MedeA UNCLE: Atomistic Studies of Crystalline Systems at Higher Scales.

Find out more by visiting the Materials Design Application Notes:

- Adaptive Crystal Structures of Au-Cu Alloy
- Structure and Bonding of Boron Carbide

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