materials design®

MedeA-UNCLE

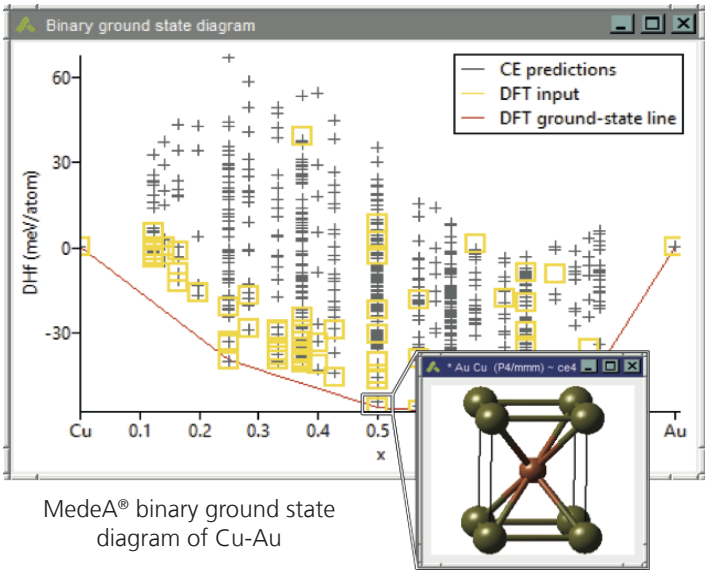
MedeA-**UN**iversal **CL**uster **E**xpansion (UNCLE) expands access to materials and properties at the meso and micro scales. Maintaining the predictive power and accuracy of first-principles Density Functional methods, MedeA-UNCLE lets you determine stable multi-component crystal structures and rank metastable structures by enthalpy of formation. Moreover, you can employ the module to explore order-disorder phenomena and phase segregation processes as a function of temperature and composition. Performing VASP first principles calculations on automatically chosen sets of small models, MedeA-UNCLE captures the configurational complexity of real materials at different temperatures by means of Monte Carlo random sampling. Tight integration with job control in MedeA® guarantees stability and fault tolerance. Graphical tools monitor progress of fully automated simulations and allow a ready-for-use visualization of results.

Key Benefits of MedeA-UNCLE:

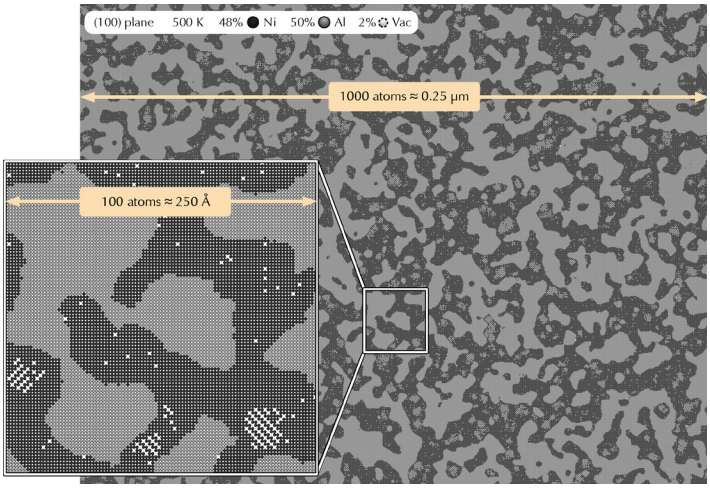
- *Models systems containing millions of atoms with DFT accuracy*
- *User-friendly setup within MedeA® Environment*
- *Workflow-based automation of cluster expansion refinement*
- *Efficient handling of hundreds of input structures*
- *Intuitive graphical analysis and visualization*
- *Split and restart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

Computational Characteristics:

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



MedeA® binary ground state diagram of Cu-Au



D Lerch, O Wieckhorst, G L W Hart, R W Forcade, and S Müller, *Model. Simul. Mater. Sci. Eng.* 17, (2009): 055003.

Properties From MedeA-UNCLE:

- *Structures of stable phases*
- *Vacancy concentrations*
- *Miscibility*
- *Random mixing energy*
- *Phase stability as a function of temperature and concentration*
- *Solubility*
- *Order-disorder transition temperature*
- *Micro structure*

Required MedeA® Modules

- *Core MedeA® Environment*
- *MedeA® JobServer and TaskServer*
- *MedeA-VASP*

*Visit our website **www.materialsdesign.com** or contact your local Materials Design office for further information.*

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