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Structural stability of alloys : ab initio and phenomenology

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The prediction of phase stability trends and phase diagrams of multi-component complex alloys is undoubtedly the Holy Grail of alloy physics and materials properties simulation. First-principles results of alloy energetics and phase diagrams can appropriately supplement thermodynamic databases that are used within the phenomenological CALPHAD approach for predicting the stability properties of complex multi-component alloys. Routine energy minimization of alloys stability within *ab initio* methodology provides input to CALPHAD in terms of heats of formation and transformation for alloys exhibiting various crystalline structures and any chemical configuration. Additionally, *ab initio* energetics combined with a statistical treatment provides the necessary thermodynamic information for subsequent assessments similar to those performed with experimental data within CALPHAD. Following an overview of the first-principles and phenomenological methodologies, examples of both aspects of the interfacing will be presented with applications to multi-component alloys. Validity of this interfacing and its relevance to alloy design will be discussed. Finally the usage of these results in meso-scale modeling of microstructure evolution will be discussed.

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Lundi 30 Juin 2008 à 10h30

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