Computational Thermodynamics and Its Applications on New Materials Design

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Abstract

Computational thermodynamics is the core of materials genome initiative (MGI) and integrated computational materials engineering (ICME). MGI and ICME are the most modern approach for new materials development and innovative process optimization. In this presentation, computational thermodynamics approaches including CALPHAD (calculation of phase diagram) method and density functional theory (DFT) method will be introduced. Few practical examples of new materials development based on computational thermodynamics will be presented, as follows: (1) high-performance free-cutting steel; (2) refractory high-entropy superalloy; (3) anode materials in Li-ion batteries; (4) low-temperature Pb-free solder. The computational thermodynamics and its applications for developing new multi-component materials in various fields are demonstrated.

Keywords: *CALPHAD; ab initio calculations; alloy design; steel; high-entropy alloy; Li-ion batteries; low-temperature Pb-free solder.*