First-principles Calculations and Thermodynamic Modeling of the Ni-Re-Y system

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Introduction
Ternary modeling using the CALculation of PHAse Diagram (CALPHAD) technique requires knowledge of the constituent binaries. The Ni-Y and the Ni-Re systems had previously been modeled. First-principle calculations were performed for pure Re, pure Y, and the hexagonal laves C14 compound, Re2Y, that exists in the system. The results were coupled with the CALPHAD technique to predict a model of the Re-Y and Ni-Re-Y systems.

Aim
Ni-base superalloys are incredibly important because they can operate at temperatures upwards of 70% of their melting temperatures. Future improvement of these alloys requires multi-component alloys at extremely specific compositions to be designed that often have high experimental costs. The CALculation of PHAse Diagram (CALPHAD) technique meets this challenge by extrapolating data from simple binary systems to higher order systems.

First-principles : 0K Method
Special quasirandom structures (SQS's) mimic correlation functions of perfectly random structures for the first several nearest neighbor shells.

Finite temperatures: Method
•Helmholtz free energy as a function of temperature

F(V,T) = E(V) + F_{vb}(V,T) + F_{vib}(V,T)

•Quasi-harmonic approach:
Vibrational contribution is calculated at several volumes and then minimized as a function of equilibrium volume

Pure elements → Binary → Ternary → Multicomponent

The CALPHAD Method
Thermochemical data: enthalpy, entropy, heat capacity, activity
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Phase equilibria: liquidus, solidus, phase boundary
Gibbs Energy of Individual Phases

Conclusion
First-principles calculations were coupled with the CALPHAD technique to model the Re-Y system. The Re-Y and Ni-Re-Y systems have been added to the Ni-base superalloy database in the CALPHAD community.

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