A combined thermodynamic and first-principles approach to predict TCP phase formation, using the Re-W and Re-Ta systems as examples

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The addition of refractory elements greatly enhances the creep resistance of single crystal superalloys, especially Re - but also W - has proven to be very effective in this way. The downside is that greater contents of refractory elements promote the formation of topologically closed packed phases (TCP), which are detrimental to materials performance. Optimisation of alloys therefore means balancing the concentration of TCP formers against other elements. As TCP formation is a very slow process, it is not easily assessable by experiments, therefore guidelines for critical amounts and combinations of TCP forming elements are needed. In order to derive robust prediction of TCP formation, which has to include information about TCP phase fractions and solvus temperatures, understanding the thermodynamic stability of TCP phases is required.

In this work we demonstrate how a combined first principles/CALPHAD approach can be used to gain fundamental insight into this problem. For this we chose the binary Re-Ta and Re-W systems, because both contain not only one of the most often encountered TCP phase –the sigma phase- but also a number of other TCP phases. These serve as prototypes for the investigation of these phases in more complex higher order systems.

The Compound Energy Formalism (CEF) was applied to describe stable and metastable TCP phases, with the enthalpies of formation being obtained from DFT (density functional theory) results. From these results site occupancies were calculated. The results show that in the investigated systems the TCP phases are stabilised by entropic effects. Phase diagrams predicted from these results are compared with experimental ones and other experimental data. Finally the way to extend the approach to higher order systems is discussed.