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First *ab initio* calculation of a σ-phase in a ternary system: Cr-Mo-Re

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For the first time, the enthalpies of formation at 0 K of all the ordered configurations in a ternary σ-phase, *i. e.* 3^5=243 configurations, have been calculated using the electronic first principles methodology. The Density Functional Theory (DFT) method has been used in the Generalized Gradient Approximation (GGA), with Projector Augmented Wave (PAW) pseudopotentials, as implemented in Vienna ab initio Simulation Package (VASP).

The Cr-Mo-Re system has been judiciously chosen to be investigated since the two binary Cr-Re and Mo-Re σ-phase are known for showing inverse Re sites preference: low coordination number (CN) sites in Cr-Re [1] and high CN in Mo-Re [2]. Occupancies of the inequivalent sites have been computed as a function of composition and temperature using the only configurational entropy, in the Bragg-Williams approximation.

The results show that the Cr-Mo-Re σ-phase presents a miscibility gap at low temperature and that the Gibbs energy surface is convex above ~750K. Re site preference is shown to change progressively in the ternary field when passing from Mo-Re to Cr-Re binary borders. The relative stability of this ternary phase will be discussed by analyzing the crystallographic parameters and the electronic properties features.

References

[1]   M. Palumbo, T. Abe, C. Kocer, H. Murakami, H. Onodera, in preparation
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