Thermodynamic Database Comparision between First-principles Calculations and Neural Network Potential

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Platinum-Rhodium (Pt-Rh) system is one of the prominent alloys used for the high temperature and high corrosion applications. It exhibits single solid solution phase across the composition rage up to 2000K. Thermodynamic database for Pt-Rh is very important for the development of the new alloys compositions. However, it is often time consuming and costly due to several experimental data are needed. Using first-principles calculations, the process can be accelerated but still need a lot of computational resources. With the emergance of machine learning, the same data can be obtained for a fraction of resources required by first-principles calculations. In this work, we compared the results of thermodynamic database developed using first-principles calculations and neural network machine learning potential[1].

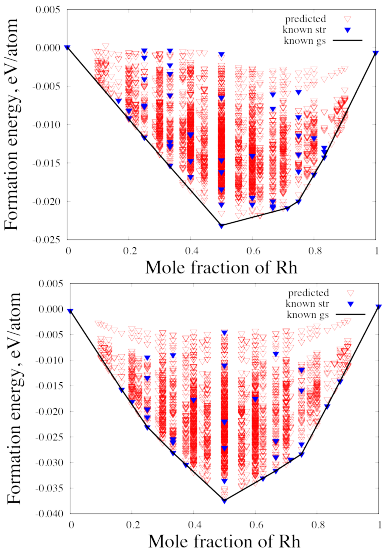

Figure 1: CEM results for DFT (top) and ML (bottom).

Cluster expansion method[2] (CEM) has been performed to obtaine the stable ground state structures for the Pt-Rh system. Figure 1 shows the cluster expansion results for both appracheds. The results are mostly in agreement with the previous literatures. Special quasirandom structures[3] (SQS) are used for the calculation of disordered structures. Finite temperature properties for SQS are performed for using both appraches to obtain the interaction parameters. Figure 2 compared the calculated phase diagram from machine learning potentials with the first-principles calculation data. The PtRh phase stability is only about 50 K differences while $PtRh_3$ is around 100 K. The results seem promising since the computational times required for machine learning potentials are lower by two to three orders of magnitude.

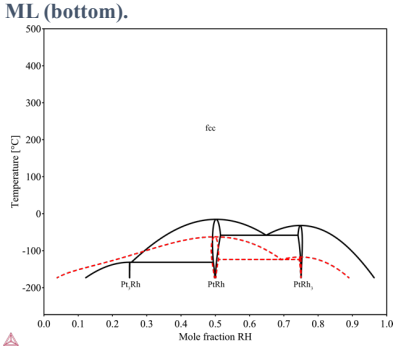

Figure 2: Calculated phase diagram from ML (solid) compared with DFT (dash).

References

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2. Sanchez, J.M., *Phys. Rev. B*, **2010**, 81, 224202.
3. Zunger, A. et al., *Phys. Rev. Lett.*, **1990**, 65, 353-356.