Short-range order in high entropy alloys: Thermodynamic modeling and application to Nb-Ti-V-Zr system

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Shanker Kumar

Department of Metallurgical Engineering

Indian Institute of Technology (Banaras Hindu University)

Varanasi-221005, India

Roll No. 17141011 **2023**

Chapter 7

Summary And Suggestions For Future Work

HEAs represent a promising class of materials with unique properties that have the potential to revolutionize various industries. Research is needed to understand and exploit their properties fully. Computational thermodynamics (CT) is an important tool for understanding the phase stability and thermodynamic properties of high entropy alloys (HEAs). The most important task of CT is the correct representation of the Gibbs energy of individual phases. Physically sound models such as CVM, which account for short-range order, are used in the current investigation. The reassessment of binary phase diagrams establishes the importance of the CVM model. Thermodynamic properties of the higher-order system using the CVM model are performed in this work. Theoretical modeling is used to investigate SRO in HEAs. The effect of temperature and composition on thermodynamic properties and SRO is established in this thesis.

However, further research is needed to improve the accuracy of computational models and integrate them with experimental methods to understand the properties of HEAs fully. To verify the values of thermochemical data obtained using DFT, experimental techniques such as DTA/DSC can be used. Experimental techniques such as X-ray and neutron scattering, transmission electron microscopy, and atom probe tomography can be used to investigate SRO in HEAs. The scattering data analysis can provide information on the degree and nature of SRO in HEAs. This study reveals the importance of SRO in dealing with composition of an alloy with varying temperature. Experiments can be performed to very this hypothesis. In this work the thermodynamic properties of ternary and quaternary system is calculated using the assessed data of binary system. The assessment of ternary and quaternary system with experimental values of thermochemical data is essential to obtain more correct values of CECs, that can be used to further improve alloy design criteria.

The framework used in the present thesis can be extended to fcc and hcp also. The present framework is limited to quaternary system only. This framework can be extended to quinary or higher order system.

In conclusion, experimental investigation of SRO in HEAs is critical for understanding their properties and optimizing their performance for specific applications. Advanced experimental techniques and analysis methods need to be developed to investigate SRO in HEAs at higher spatial resolution and with higher accuracy. Further research is needed to understand the underlying mechanisms of SRO in HEAs and its dependence on processing parameters and defect structures.

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