Structural, mechanical, and electronic properties of BCC refractory binary alloys: A first-principles study

S. Bijjala[a], P. Kumar[a], and Susan R. Atlas[b,c]
[a]Department of Mechanical Engineering, University of New Mexico, Albuquerque, NM 87131
[b]Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, NM 87131
[c]Department of Physics and Astronomy and Center for Quantum Information and Control, University of New Mexico, Albuquerque, NM 87131

Abstract
Multicomponent refractory high-entropy alloys (RHEAs) with compositional complex microstructure can offer superior high-temperature mechanical properties compared to the conventional alloys. However, exploring the vast number of RHEAs compositions and their respective properties is a significant challenge. First-principles density functional theory (DFT) methods provide a quantum-level approach for exploring the vast design space offered by complex RHEA systems. To enable the efficient exploration of the combinatorically-complex design space of 5+ element RHEA using machine learning (ML) techniques, we have performed DFT calculations on the relevant unary and binary systems. This approach takes advantage of the known correlation of results obtained from simpler systems in predicting properties of complex alloys [1]. The atomic and electronic insights derived from these composition–structure–property relationships enable the identification of key features/principles for ML design strategies. We present results for structural and electronic properties (lattice constants and formation energies) and mechanical properties (elastic constants) calculated for MoNb, MoTa, MoW, NbTa, WNb and WTa BCC refractory binary alloys. Initial benchmarking studies were performed to establish the methodology and computational parameters for Mo, Nb, Ta and W. Computed properties using d, p and s valence electron-norm-conserving pseudopotentials [6] and using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation energy density functional [7] agree well with other theoretical calculations and with experiment. Special quasi-random structure (SQS) supercells [2,3] were used to represent the disordered binary alloys. The effect of strain due to random arrangement of atoms of different atomic radii in SQS supercells was studied by considering spin and relaxation effects on structural properties. Elastic constants were calculated using density functional perturbation theory with strain perturbation [4]. All calculations were performed using the Abinit DFT electronic structure code [5]. We discuss the computed results in the context of experimental observations.

We would like to thank the UNM Center for Advanced Research Computing, supported in part by the National Science Foundation, for providing the high-performance computing, large-scale storage and visualization resources used in this work. This work was supported in part by NASA EPSCoR Grant # 80NSSC21M0171.

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