Influence of the center atom in BCC MoTaVNbW high entropy alloys

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The structural properties and the influence of Nb and W as center atoms in BCC structures of the high entropy alloy MoTaVNbW were examined by using density functional theory. Results indicate that there is "little or no change" in the lattice parameter of the MoTaVNbW in the BCC structure with Nb or W as the center atom. The change in middle atom does have an effect on the bulk modulus and by consequence on the melting temperature of the materials.

I. INTRODUCTION

Recently, high entropy alloys (HEA) became the topic of many research projects. They show promising properties and could be used in many different applications. HEAs are typically composed of more than five metallic elements in equal or near-equal atomic ratios, and interestingly they tend to form solid solution structure (mainly FCC and/or BCC) rather than multiple intermetallic compounds as expected from general physical metallurgy principle [1]. In this paper, density functional theory (DFT) is used to take a closer look at MoTaVNbW high entropy alloys with a BCC structure [2]. Two different BCC structures are examined. The first one has Nb as the body centered atom, the second has W as body centered atom. The influence of this atom on the optimal lattice parameter and bulk modulus is calculated and investigated .

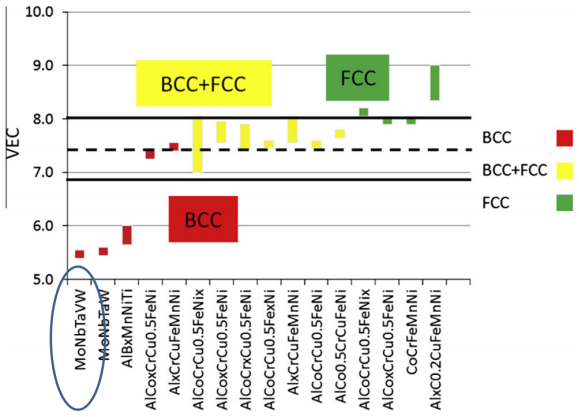

FIG. 1. Different high entropy alloys and their possible unit lattices

II. COMPUTATIONAL DETAILS

We have used the first-principles pseudopotential plane wave method based on DFT incorporated into the Quantum Espresso package [3] with PBE exchange-correlation functional [4] for all calculations. Wave functions and charge density were expanded in a plane wave basis up to a kinetic-energy cutoff of 37 and 148 Ry, respectively, which are sufficient to obtain converged results.

A 2x2x2 supercell of MoTaVNbW was created and visualized with VESTA [5]. Two cases were investigated: a BCC structure with Nb as the center atom and the other with W as the center atom.

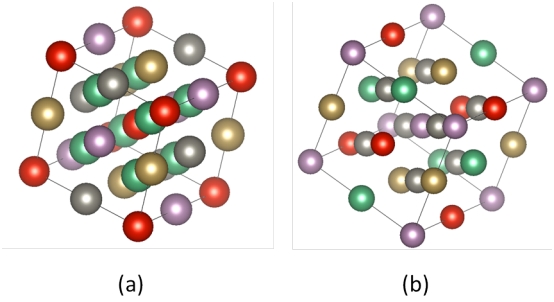

FIG. 2. Visualization of the cif files in VESTA. (a) Nb as middle atom, (b) W as middle atom

A. Cif files

A cif file describes the crystallographic nature of the investigated materials. In this case the two materials are both BCC materials with five different elements: Mo, Ta, V, Nb and W. These elements are used in a BCC structure based on the results of *Y. Zhang et al.* shown in figure 1 [2].

Two cif files are created with different atoms at the center positions of the BCC structures; Nb and W. Both files are visualized using VESTA as shown in figure 2. The lattice parameters are not optimal in this case.

B. Convergence testing

The cif files were transformed to Quantum Espresso input files. After convergence testing a k-mesh of 9x9x9, an ecutwfc-value of 37 and an ecutrho-value of 148 were found as the convergence settings to obtain sufficiently correct results.

III. DFT RESULTS

A. Estimation of the lattice parameters

1. *Rough estimation of the lattice parameter*

In order to find the correct lattice parameters of the 2x2x2 supercells shown in figure 2. A volume optimization was conducted on both structures. For both structures the energy was the lowest for a lattice parameter of 6.2. This means that for the regular unit cell this value becomes 3.1 since 2x2x2 supercells were used for the calculations. Figure 3 shows the date for the case where Nb is the center atom.

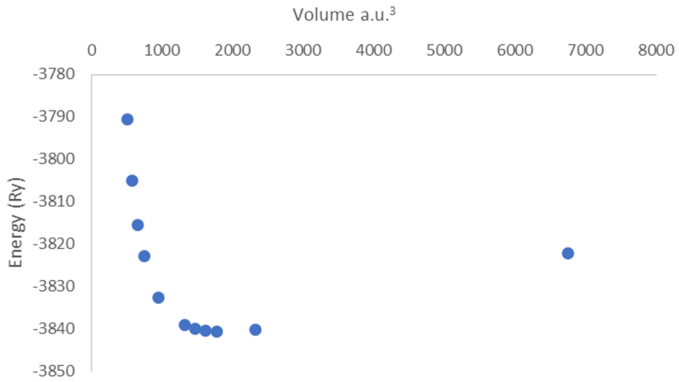

FIG. 3. Energy versus volume for Nb as center atom

2. *More exact estimation of the lattice parameter*

Based on the previous value of 6.2, determined in section 1, a more exact estimation of the lattice parameter is made by slightly varying the volume around this point. The energy versus volume graphs can be seen in figure 4. For the Nb case the optimal lattice parameter becomes 6.5 while for the W case it becomes 6.4. This results in 3.25 and 3.2 respectively for the unit cells.

B. Estimation of the bulk modulus

The graphs in figure 4 made it possible to estimate the bulk modulus of both materials by taking the second derivative. In the case of Nb as middle atom the bulk modulus is $4 * 10^{-6} Ry/a.u.^2$, while for W as middle atom the bulk modulus is $5 * 10^{-6} Ry/a.u.^2$. Since the bulk modulus is roughly related to the melting temperature, it can be concluded that the middle atom of the BCC structure in HEA has an influence on the melting temperature.

IV. CONCLUSION

It can be concluded that the middle atom in a BCC MoTaVNbW high entropy alloy has an influence on both the lattice parameter and the bulk modulus. Nb as middle atom expands the lattice slightly compared with a structure containing W as body centered atom. The bulk modulus which is related with the melting temperature is larger for the W case, indicating that the melting temperature is higher.

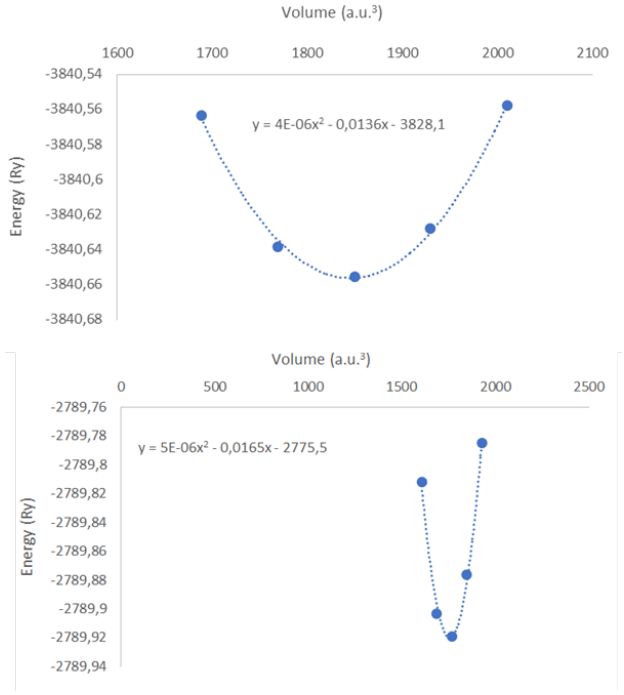

FIG. 4. Energy vs volume for Nb (top) and W (bottom)

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