Examination of the Mechanical and Phase Properties of the Refractory High Entropy Alloy ReMoNbTaV

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Consortium for Innovation in Manufacturing & Materials

Research Highlights

- Calculations were done by the SSOS method which can achieve the same accuracy as the large supercell for the RHEAs but is more efficient in consideration of computational cost
- Properties of RHEA ReMoNbTaV with three refractory elements: Niobium(Nb) , Tantalum (Ta), and Vanadium (V)
- High temperature performance and strength of the material can lead to various industrial applications

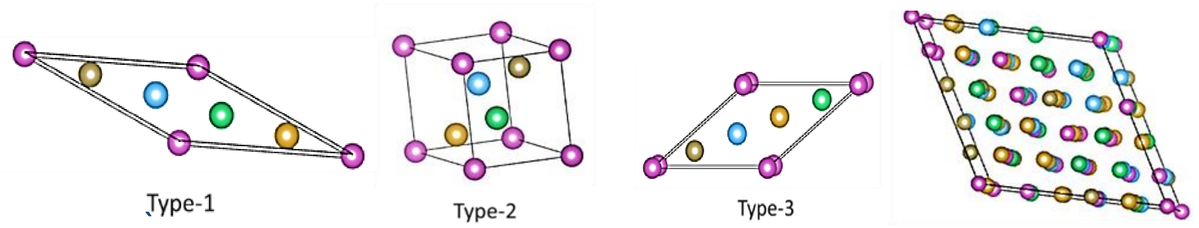
Context

- This project contributes to CIMM research in the exploration of a new type of high entropy alloy made with refractory elements Nb, Ta, and V
- The refractory elements in HEAs may lead to a better high-temperature performance, which makes RHEAs highly applicable for aerospace industry, cryogenics, hard coating industries and high temperature refractory applications

Computational Methods

- The structure of ReMoNbTaV was optimaized by The Vienna Ab Initio Simulation Packages (VASP) based on Density Functional Theory. The atomic structure of ReMoNbTaV with BCC structure of 100 atoms was created in Material Studio 7.0.
- The Equation of state (EOS) program for fitting energy-volume data was used to calculate the bulk modulus and the atomistic simulation tool MedeA as well as Voigt-Reuss-Hill (VRH) methods were used to calculate the other mechanical properties of ReMoNbTaV.
- The phase diagram was calculated by The Thermo-Calc-2019 software and the scheil solidification simulation as well as the total latent heat of ReMoNbTaV was found using the TCHEA1 database calculations. The RHEA ReMoNbTaV was composed of 20 percent each of Re, Mo, Nb, Ta, and V.

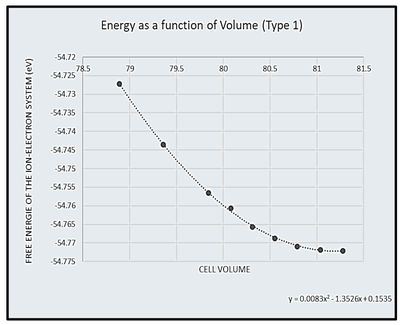
The SSOS models (type-1 to type-3) with five elements (represented by different colors) used for calculations and type-4 supercell for comparison

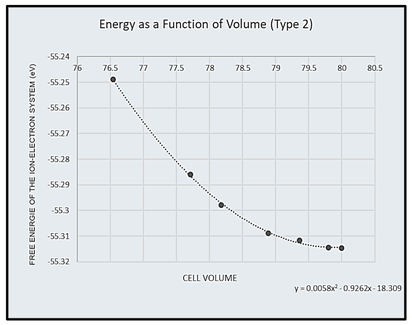


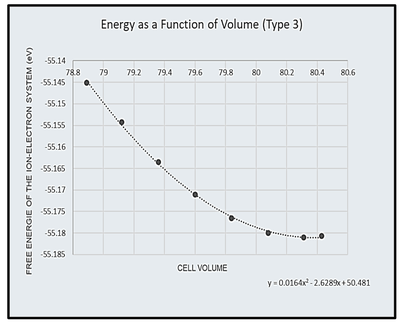
12345	12435	12543	13245	13425	14235
12354	12453	12534	13254	13524	14325

12 Configurational Arrangements

Results







- The second-degree polynomial curve is fitted and the equation is used to calculate mechanical properties such as the Bulk Module

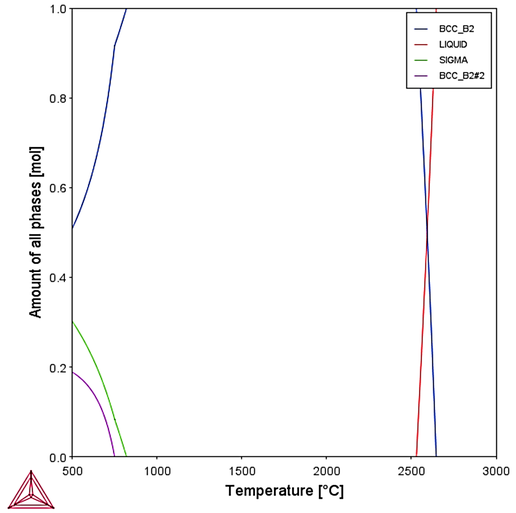
	Type 1	Type 2	Type 3	Type 4
Ratio with Minimal Energy	1.010	1.004	1.006	1.009
Average Energy of Configurations per-atom	-10.98 ev	-11.06 ev	-11.03 ev	-10.97 ev

- The average of calculated properties from type 1 to type 3 were taken to calculate the properties of RHEA with SSOS method
- The average energy of configurations using SSOS compared to the supercell is similar, assuring the accuracy of the method

ReMoNbTaV	Bulk module (GPa)	Shear module (GPa)	Young's module (GPa)	Poisson ratio (a.u)	Pugh's ratio (a.u)	Vicker's hardness (Gpa)
Calculation using SSOS	232.81	93.94	248.22	0.3221	2.487	8.21

- After bulk (B) and shear moduli (G) are achieved, Young's modulus (E), Pugh's ratio (B/G), and Poisson's ratio (v) can be predicted
- E = 9BG /(3B + G)
- v = 3B − 2G/(2(3B + G))
- B/G = B/G
- The high Bulk module indicate that the alloy is highly resistant to volume change under compression while the large Shear module indicate great resistance to reversible deformations
- The relatively high Young's module indicates that the alloy is stiff and not prone to deformation under large elastic loads
- Since the Poisson ratio is greater than 0.26 and the Pugh's ratio is greater than 1.75, the alloy is considered to be ductile
- The alloy is considered hard as seen from Vicker's hardness

Phase Diagram of ReMoNbTaV



- BCC is the only stable phase of RHEAs at high temperature
- Melting point of the alloy is at about 2600 ℃ due to presence refractory elements

Conclusions

- The alloy ReMoNbTaV showed stable BCC structure when the temperature is above 1000 ℃ and displayed high thermal stability showing promising applications in industry
- The SSOS method showed promising results seen from the energy/volume curves and the analysis of the different configurations compared to the 100 super-cell calculations.
- The mechanical properties of the alloy showed it to be highly resistant to compression, rigid, stiff, and ductile which makes the alloy desirable for industrial purposes.

Next Steps

- Experiment with different combinations of refractory elements for specific desired properties
- Substitute or eliminate a particular element to analyze the function of each element in the alloy in relation to its properties

Acknowledgements

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