World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:15, No:06, 2021

First Principal Calculation of Structural, Elastic and Thermodynamic Properties of Yttrium-Copper Intermetallic Compound

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Abstract : This work investigates the equation of state parameters, elastic constants, and several other physical properties of (B2-type) Yttrium-Copper (YCu) rare earth intermetallic compound using the projected augmented wave (PAW) pseudopotentials method as implemented in the Quantum Espresso code. Using both the local density approximation (LDA) and the generalized gradient approximation (GGA), the finding of this research on the lattice parameter of YCu intermetallic compound agree very well with the experimental ones. The obtained results of the elastic constants and the Debye temperature are also in general in good agreement compared to the theoretical ones reported previously in literature. Furthermore, several thermodynamic properties of YCu intermetallic compound have been studied using quasi-harmonic approximations (QHA). The calculated data on the thermodynamic properties shows that the free energy and both isothermal and adiabatic bulk moduli decrease gradually with increasing of the temperature, while all other thermodynamic quantities increase with the temperature.

Keywords : Yttrium-Copper intermetallic compound, thermo_pw package, elastic constants, thermodynamic properties
Conference Title : ICAMMP 2021 : International Conference on Advanced in Materials and Manufacturing Processes
Conference Location : Istanbul, Türkiye
Conference Dates : June 28-29, 2021