World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:9, No:01, 2015

Ab Initio Studies of Structural and Thermal Properties of Aluminum Alloys

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Abstract : We present the results of a systematic and comparative study of the bulk, the structural properties, and phonon calculations of aluminum alloys using several exchange–correlations functional theory (DFT) with different plane-wave basis pseudo potential techniques. Density functional theory implemented by the Vienna Ab Initio Simulation Package (VASP) technique is applied to calculate the bulk and the structural properties of several structures. The calculations were performed for within several exchange–correlation functional and pseudo pententials available in this code (local density approximation (LDA), generalized gradient approximation (GGA), projector augmented wave (PAW)). The lattice dynamic code "PHON" developed by Dario Alfè was used to calculate some thermodynamics properties and phonon dispersion relation frequency distribution of Aluminium alloys using the VASP LDA PAW and GGA PAW results. The bulk and structural properties of the calculated structures were compared to different experimental and calculated works.

Keywords : DFT, exchange-correlation functional, LDA, GGA, pseudopotential, PAW, VASP, PHON,phonon dispersion
Conference Title : ICAM 2015 : International Conference on Advanced Materials
Conference Location : Jeddah, Saudi Arabia
Conference Dates : January 26-27, 2015