

Structural, Electronic and Mechanical Properties of C14-Mg₂ RE (RE=Eu, Er, Tm, Yb and Lu) Laves Phases: A DFT Study

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Abstract: The Pseudo-Potential Density Functional Theory (PP-DFT) method is applied to investigate the structural, electronic and mechanical properties of C14-Mg₂ RE Laves phases, with RE being Eu, Er, Tm, Yb and Lu. The predicted cell parameter and c/a ratio of each compound are in good agreement with experimental and theoretical results. Moreover, the studied alloys exhibit a metallic character, which is attributed to the presence of Mg atoms in the C14 Laves phase. Also, the formation of C14-Mg₂ RE is found to be controlled by the hybridisation between Mg p states and RE-d and f states. From a mechanical property analysis, the studied alloys are found to be mechanically stable. The Mg₂ Lu compound exhibits higher ductility, while Mg₂ Er exhibits the smallest one. Finally, Mg₂ Yb is found to be more anisotropic than other phases.

Keywords : A DFT calculations, B Magnesium based Laves phases, C Density Functional Theory (DFT), D Mechanical properties, E Electronic properties