Chinese Journal of Physics

Volume 57, Issue 1, 2019, Pages 146-156

Structural, Electronic and Mechanical Properties of C14-Mg 2 RE(RE=Eu, Er, Tm, Yb and Lu) Laves Phases: A DFT Study

A. Zahague, B. Lagoun, A. Legris, R. Besson, L. Rabahi, D. Bradai

Abstract: The Pseudo-Potential Density Functional Theory (PP-DFT) method is applied to investigatethe structural, electronic and mechanical properties of C14-Mg 2 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 metalliccharacter, which is attributed to the presence of Mg atoms in the C14 Laves phase. Also, theformation of C14-Mg 2 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 mechanicallystable. The Mg 2 Lu compound exhibits higher ductility, while Mg 2 Er exhibits the smallest one.Finally, Mg 2 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