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A systematic DFT study of $(Ti_{3/2}RE_{1/2})AlC$ alloys: A new database for adjustable mechanical and electronic properties

C. Meftah [a,b], N. Iles [c,*], L. Rabahi [b,d], M. Gallouze [b], H.I. Feraoun [e], M. Drir [b]

[a] Département de physique, Faculté des sciences, Université M'Hamed BOUGARA de Boumerdès (UMBB), 35000 Boumerdès, Algeria
[b] Laboratoire de physique théorique (LPT), Faculté de physique, Université des Sciences et Technologies Houari Boumediène (U.S.T.H.B), BP 32 El Alia, 16111 Bab-ezzouar, Alger, Algeria
[c] Laboratoire de Physique des Couches Minces et Matériaux pour l'Electronique, LPCMME Université Oran 1 Ahmed Ben Bella, Oran, Algeria
[d] Research Center in Industrial Technologies CRTI, P. O. Box 64, Cheraga 16014, Algiers, Algeria
[e] Unité de Recherche Matériaux et Energies Renouvelables – URMER, Université de Tlemcen, Algeria

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ABSTRACT

In this study, ab initio calculations based on Pseudo-Potential Density Functional Theory (PP-DFT) method are carried out in order to highlight the partial substitution effect of Rare Earth (*RE*) elements in the well-known 211-*MAX* phase of Ti_2AlC. The considered elements are Y, Sc and *RE* = La, Ce, Pr, Nd, Sm, Eu, Gd leading to $(Ti_{3/2}RE_{1/2})AlC$ alloys. According to the obtained results, the $(Ti_{3/2}RE_{1/2})AlC$ alloys are significantly less compressible under uniaxial stress along x and z axes. They exhibit high resistance to shearing along <001> direction. In addition, the calculated heat capacity for $(Ti_{3/2}RE_{1/2})AlC$ alloys increases with respect to the temperature, a maximum is found in the temperature range 200–300 K. Localized states occur in $(Ti_{3/2}RE_{1/2})AlC$ alloys due to the f states filling of the rare earth elements. The magnetic moment of $(Ti_{3/2}RE_{1/2})AlC$ compounds increases according to $4f^n$($n=2$ for Ce to $n=7$ for Gd) filling. Our findings provide a theoretical database for new tunable properties of $(Ti_{3/2}RE_{1/2})AlC$ alloys.

1. Introduction

The *MAX* phases are outstanding alloys classified between hard ceramics and metals with unusual properties. They are elastically rigid, good thermal and electrical conductors, resistant to the chemical environment and stable at high temperatures. They have good magnetic and mechanical properties, low thermal expansion coefficients, a low density and a good machinability [1–7]. These unique properties make *MAX* phases materials interesting for various applications as coating materials, engine parts, melting furnaces, low-friction electrical contacts [8–11].

The Ti_2AlC alloy is known to have higher physical properties when compared to the other alloys of *MAX* phase family as well as its binary counterpart TiAl [6,7,12–14]. This alloy has low-cost constituents, an excellent oxidation resistance and a good electrical conductivity [9,15]. It possesses a good thermodynamic and mechanical stability [16,17]. Moreover, interesting properties of its two-dimensional (2D) derivatives, called *MXenes*, have been experimentally synthesized by removing chemically the Al layer from Ti_2AlC compounds [18,19]. Solid solution obtained by substituting Ti, Al and C atoms improves remarkably the physical and chemical properties of Ti_2AlC. Fang et al. studied the effect of Nb addition in Ti_2AlCr [20]. They reported results on phase composition and mechanical properties of high-C $Ti_{46}Al_{2.6}C$ (at. %) alloy reinforced by Ti_2AlC particles. The formation of Ti_2AlC particles improves the strength, strain, wear resistance and the high-temperature creep resistance in TiAl alloys [21–25]. Yu et al. showed that oxidation mechanisms and kinetics in fine-grained (FG) and coarse-grained (CG) Ti_2AlC are controlled by the grain size of Ti_2AlC [26]. The faster is the oxidation process, the greater is the grain size. Other experimental studies reported that Ti_2AlC and Ti_3SiC_2 are potential candidates for high temperature nuclear applications [27–31]. In their study, Bentzel et al. focused on the interaction of Ti_2AlC, Ti_3AlC_2, Ti_3SiC_2 and Cr_2AlC with Pd at 900 °C [32]. They clearly showed that Ti_2AlC is a promising candidate for high temperature applications. Recently, Xie et *al.* fabricated a Textured Grain (TG) composite of Ti_2AlC by using a Hot-Pressing sintering process. New mechanical properties are highlighted. The measured average fracture toughness of TG samples is about 30% higher than untextured Coarse Grain (CG) samples. Flexural strength is almost

* Corresponding author. Oran 1 university, Oran, Algeria.
E-mail address: n_ilesdz@yahoo.fr (N. Iles).

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