Retraction notice to: A theoretical investigation on the electron structures of Al-based intermetallic compounds [Arch. Metall. Mater. 58 (2013) 1023-1027]

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The reason of retraction is: this article was published under different titles, with different authorship, and minor alterations to the text elsewhere simultaneously.

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RETRACTED

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A THEORETICAL INVESTIGATION ON THE ELECTRON STRUCTURES OF Al-BASED INTERMETALLIC COMPOUNDS

TEORETYCZNE BADANIA STRUKTUR ELEKTRONOWYCH ZWIĄZKÓW MIĘDZYMETALICZNYCH NA BAZIE ALUMINIUM

Theoretical investigations were performed to study on alloying stability, and electronic structure of ($AlCu_3$, $AlCu_2Zr$ and $AlZr_3$). The results show that the lattice parameters obtained after full relaxation of crystalline cells are consistent with experimental data, and these intermetallics have a strong alloying ability and structural stability due to the negative formation energies and the cohesive energies. The further analysis find out that single-crystal elastic constants at zero-pressure satisfy the requirement of mechanical stability for cubic crystals. The calculations on Poisson's ratio show that $AlCu_3$ is much more anisotropic than the other two intermetallics. In addition, calculations on densities of states indicates that the valence bonds of these intermetallics are attributed to the valence electrons of Cu 3d states for $AlCu_3$, Cu 3d and Zr 4d states for $AlCu_2Zr$, and Al 3s, Zr 5s and 4d states for $AlZr_3$, respectively; in particular, the electronic structure of the $AlZr_3$ shows the strongest hybridization.

Keywords: intermetallic, first-principles, electron structure

Przeprowadzono teoretyczne badania stabilności stopów i struktury elektronowej $AlCu_3$, $AlCu_2Zr$ i $AlZr_3$). Obliczenia wskazują, że parametry sieci uzyskane po pełnej relaksacji komórek krystalicznych są zgodne z danymi eksperymentalnymi. Związki międzymetaliczne wykazują silną zdolność tworzenia stopów i stabilność strukturalną z powodu ujemnej energii tworzenia i energii spójności. Dalsze analizy wykazały, że stałe elastyczności pojedynczych kryształów przy zerowym ciśnieniu spełniają wymóg stabilności mechanicznej kryształów regularnych. Obliczenia współczynnika Poissona pokazują, że $AlCu_3$ posiada znacznie bardziej anizotropowe własności niż dwie pozostałe fazy mioędzymetaliczne. Ponadto, obliczenia gęstości stanów wskazują, że w tworzeniu faz międzymetalicznych biorą udział elektrony walencyjne odpowiednio: Cu na powłoce 3d dla $AlCu_3$, Cu na 3d i Zr na 4d dla $AlCu_2Zr$, oraz Al na 3s, Zr na 5s i 4d dla $AlZr_3$), w szczególności struktura elektronowa $AlZr_3$) wykazuje najsilniejszą hybrydyzację.

1. Introduction

Intermetallics involving aluminum and transition metals (TM) are known to have high resistance to oxidation and corrosion, elevated-temperature strength, relatively low density, and high melting points, which making them desirable candidates for high-temperature structural applications [1, 2]. In particular, Zirconium can effectively enhance the mechanical strength of the alloys when copper and zinc elements exist in aluminum and Al-based alloys [3]. Adding Zr in the Al-Mg alloys can effectively discard hydrogen, grain refinement, reducing pinholes, porosity and hot cracking tendency and improve its mechanical properties [4]. Many investigations have focused on the constituent binary systems, such as Al-Cu, Al-Zr, and Cu-Zr[5-10], however, there has been a lack of systematic theoretical and experimental investigations for binary and ternary system, especially for ternary alloy system.

In recent years, first-principles calculations based on the density-functional theory have become an important tool for the accurate study of the crystalline and electronic structures and mechanical properties of solids [11]. In the present study, we report a systematic investigation of the structural, elastic and electronic properties of Al-based alloys($AlCu_3$, $AlZr_3$ and $AlCu_2Zr$) by first-principles calculations, and the results are discussed in comparison with the available experimental data and other theoretical results.

2. Computational method

All calculations were performed using the Vienna ab initio Simulation Package (VASP) [12,13] based on the density-functional theory (DFT) [14]. The exchange and correlation energy was treated within the generalized gradient approximation of Perdew-Wang 91 version (GGA-PW91) [15].The interaction between the valence electrons and the ions was described by using potentials generated with Blöchl's projector augmented wave (PAW) method [16]. The PAW potential used for Al treats 3s, 3p states as valence states, and the other electron-ion interaction was described by 3d, 4s valence states for Cu, 5s, 4d ,5p valence states for Zr. A plane-wave energy cutoff was set at 450eV for $AlCu_3$ and

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