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HYDROGEN ADSORPTION ON beta-TiAl (001) AND Ni/TiAl (001) SURFACES

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SURFACE REVIEW AND LETTERS

Volume: 21 Issue: 3

Article Number: 1450034

DOI: 10.1142/S0218625X14500346

Published: JUN 2014

[View Journal Impact](#)

Abstract

In this paper, we present first principles calculations of the energetic, electronic and magnetic properties of the variant termination of TiAl (001) and Ni/TiAl (001) surfaces with and without hydrogen atoms. The calculations have been performed within the density functional theory using full-potential linearized augmented plane wave method. The generalized gradient approximation (GGA) is utilized as the exchange-correlation energy. The octahedral site is the stable absorption site of H atom in the beta-TiAl system. This absorption reduces the cohesive energy of beta-TiAl system due to increase in the lattice constant. The surface energy for both TiAl (001) terminations is calculated. The stable adsorption site of H atoms on the variant termination of TiAl (001) surface is performed. The adsorption energy of hydrogen on Ti is more energetic than that on Al. The adsorption of H atom on both terminations of H/Ni/TiAl (001) is more preferable at the bridge site. The adsorption energies are enhanced on Ni atom due to the contraction between d-Ni bands and TiAl substrate band.

Keywords

Author Keywords: TiAl; hydrogen; surface energy; LDOS; charge density

KeyWords Plus: SINGLE-CRYSTAL SURFACES; DIRECTIONAL SOLIDIFICATION; ALLOYS; ALUMINIDES; SYSTEMS

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Publisher

WORLD SCIENTIFIC PUBL CO PTE LTD, 5 TOH TUCK LINK, SINGAPORE 596224, SINGAPORE

Categories / Classification

Research Areas: Chemistry; Physics

Web of Science Categories: Chemistry, Physical; Physics, Condensed Matter

Document Information

Document Type: Article

Language: English

Accession Number: WOS:000336961600004

ISSN: 0218-625X

eISSN: 1793-6667

Citation Network

2 Times Cited

35 Cited References

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Mubarak, A. A. The elastic, electronic and magnetism structure of the MAI and M3Al (M = Fe and Ni) alloy with and without hydrogen atoms . JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS, MAR 1 2016.

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