

Accepted Manuscript

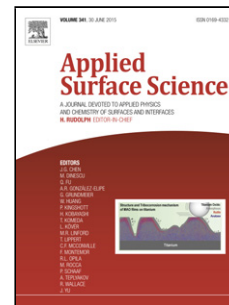
Title: Stability of the Al/TiB₂ interface and doping effects of Mg/Si

Authors: Chao Deng, Ben Xu, Ping Wu, Qiulin Li

PII: S0169-4332(17)31882-2
DOI: <http://dx.doi.org/doi:10.1016/j.apsusc.2017.06.227>
Reference: APSUSC 36427

To appear in: *APSUSC*

Received date: 12-4-2017
Revised date: 5-6-2017
Accepted date: 21-6-2017



Please cite this article as: Chao Deng, Ben Xu, Ping Wu, Qiulin Li, Stability of the Al/TiB₂ interface and doping effects of Mg/Si, Applied Surface Science <http://dx.doi.org/10.1016/j.apsusc.2017.06.227>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Stability of the Al/TiB₂ interface and doping effects of Mg/Si

Chao Deng¹, Ben Xu², Ping Wu³, Qiulin Li^{1,*}

¹Joint Laboratory of Nuclear Materials and Service Safety, Graduate School at Shenzhen, Tsinghua University, Shenzhen 518055, China

²School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

³Entropic Interface Group, Engineering Product Development, Singapore University of Technology and Design, 8 Somapah Road, Singapore 487372, Singapore

Highlights

1. The interfacial energies of Al/TiB₂ interfaces are investigated and the results support the reported grain refinement mechanisms in Al-Si alloys.
2. The segregation behaviors of the doped Mg/Si atoms to the interfaces are studied. Segregation occurs when the interface is rich in B.
3. By comparing the work of separation, we find that the interfaces will both weaken after doping Mg/Si, thus hinder the formation of TiB₂.

The Al/TiB₂ interface is of significant importance in controlling the mechanical properties of Al-B₄C composites and tuning the heterogeneous nucleation of Al/Si alloys in industry. Its stability and bonding conditions are critical for both purposes. In this paper, the interfacial energies were investigated by first-principles calculations, and the results support the reported grain refinement mechanisms in Al/Si alloys. Moreover, to improve the mechanical properties of the interface, Mg and Si were doped at the interface, and our simulations show that the two interfaces will both weaken after doping Mg/Si, thus the formation of TiB₂ is inhibited. As a result, the processability of the Al-B₄C composites may be improved. Our results provide a theoretical basis and guidance for practical applications.

Key words: First-principles calculation; Al/TiB₂ interface; Al-B₄C composites; Grain refining

I. INTRODUCTION

The interface between metals and ceramics plays a vital role in the design of materials ranging from macroscale structural composites to functional thin films, as well as nanoscale electronic devices. Al/TiB₂ interface forms when Ti is added in producing Al-B₄C composites or Al-Ti-B refiner is added when producing Al or Al/Si alloy^[1-5]. It is commonly believed that the interface

Download English Version:

<https://daneshyari.com/en/article/5347386>

Download Persian Version:

<https://daneshyari.com/article/5347386>

[Daneshyari.com](https://daneshyari.com)