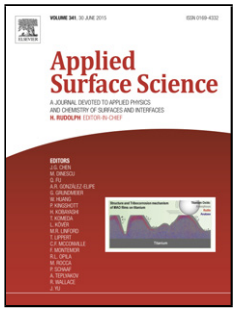

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PII: S0169-4332(17)31882-2
DOI: http://dx.doi.org/doi:10.1016/j.apsusc.2017.06.227
Reference: APSUSC 36427

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 Sciencehttp://dx.doi.org/10.1016/j.apsusc.2017.06.227

Stability of the Al/TiB_2 interface and doping effects of Mg/Si

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Highlights
1. The interfacial energies of Al/TiB_2 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 TiB_2.

The Al/TiB_2 interface is of significant importance in controlling the mechanical properties of Al-B_4C 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 TiB_2 is inhibited. As a result, the processability of the Al-B_4C composites may be improved. Our results provide a theoretical basis and guidance for practical applications.

Key words: First-principles calculation; Al/TiB_2 interface; Al-B_4C 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/TiB_2 interface forms when Ti is added in producing Al-B_4C composites or Al-Ti-B refiner is added when producing Al or Al/Si alloy [1-5]. It is commonly believed that the interface