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Investigation on AlP as the heterogeneous nucleus of Mg_2Si in Al–Mg_2Si alloys by experimental observation and first-principles calculation

Jiayue Sun[a], Chong Li[a*], Xiangfa Liu[b], Liming Yu[a], Huijun Li[a], Yongchang Liu[a**]

a. State Key Lab of Hydraulic Engineering Simulation and Safety, School of Materials Science and Engineering, Tianjin University, Tianjin 300350, P.R. China

b. Key Laboratory of Liquid-Solid Structural Evolution and Processing of Materials, Ministry of Education, Shandong University, Jinan 250061, China

Abstract

The microstructural evolution of primary Mg_2Si in Al–20%Mg_2Si with Al–3%P master alloy was observed by scanning electron microscope. And the interfacial properties of AlP/Mg_2Si interface were investigated using first-principles calculations. The calculation results show that AlP(100)/Mg_2Si(211) and AlP(331)/Mg_2Si(110) interfaces can form steadily. P-terminated AlP(100)/Mg_2Si(211) interface with the largest work of adhesion (4.13 J/m^2) is theoretically the most stable. The interfacial electronic structure reveals that there are covalent Si-Al, Si-P and Mg-P bonds existing between AlP and Mg_2Si slabs. Due to the AlP particles as effective heterogeneous nucleus of Mg_2Si, primary Mg_2Si particles change from dendrite to octahedron/truncated octahedron, and their sizes decrease to ~20μm.

Keywords: AlP; Al–Mg_2Si alloys; First-principles calculation; Heterogeneous nucleus

* Corresponding author.

** Corresponding author.

E-mail address: lichongme@tju.edu.cn (C. Li), licmtju@163.com (Y.C. Liu)