

Accepted Manuscript

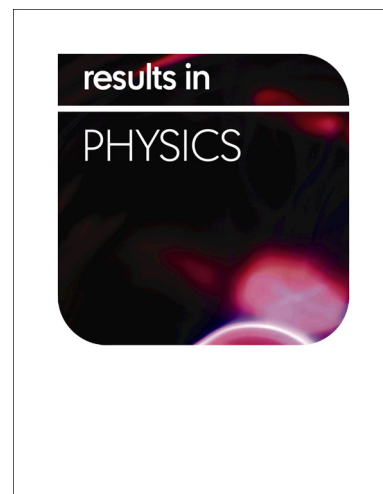
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PII: S2211-3797(17)31858-2
DOI: <https://doi.org/10.1016/j.rinp.2017.11.025>
Reference: RINP 1062

To appear in: *Results in Physics*

Received Date: 27 September 2017
Revised Date: 20 November 2017
Accepted Date: 20 November 2017



Please cite this article as: Sun, J., Li, C., Liu, X., Yu, L., Li, H., Liu, Y., Investigation on AlP as the heterogeneous nucleus of Mg_2Si in Al– Mg_2Si alloys by experimental observation and first-principles calculation, *Results in Physics* (2017), doi: <https://doi.org/10.1016/j.rinp.2017.11.025>

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Investigation on AlP as the heterogeneous nucleus of Mg₂Si in Al–Mg₂Si alloys by experimental observation and first-principles calculation

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Abstract

The microstructural evolution of primary Mg₂Si in Al–20%Mg₂Si with Al–3%P master alloy was observed by scanning electron microscope. And the interfacial properties of AlP/Mg₂Si interface were investigated using first-principles calculations. The calculation results show that AlP(100)/Mg₂Si(211) and AlP(331)/Mg₂Si(110) interfaces can form steadily. P-terminated AlP(100)/Mg₂Si(211) interface with the largest work of adhesion (4.13 J/m²) 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 Mg₂Si slabs. Due to the AlP particles as effective heterogeneous nucleus of Mg₂Si, primary Mg₂Si particles change from dendrite to octahedron/truncated octahedron, and their sizes decrease to ~20μm.

Keywords: AlP; Al–Mg₂Si alloys; First-principles calculation; Heterogeneous nucleus

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