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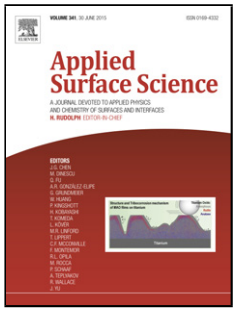

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PII: S0169-4332(17)32900-8
DOI: https://doi.org/10.1016/j.apsusc.2017.09.241
Reference: APSUSC 37320

To appear in: *APSUSC*

Received date: 14-7-2017
Revised date: 18-9-2017
Accepted date: 28-9-2017

Please cite this article as: Lan Zhang, Yongchao Zhu, Na Li, Yan Rong, Huimin Xia, Huizhong Ma, Atomistic simulation of Al-graphene thin film growth on polycrystalline Al substrate, Applied Surface Science https://doi.org/10.1016/j.apsusc.2017.09.241

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Atomistic simulation of Al-Graphene thin film growth on polycrystalline Al substrate

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Highlights

- We performed a molecular dynamics simulation of the growth of Al-Graphene composite coatings on polycrystalline Al substrate for the first time.
- The diffusion behaviors and growth process of Al adatoms on polycrystalline surface are investigated in detail, which give rise to the volmer-weber growth mode.
- The effects of the reinforcing phase in the deposition process are firstly studied in atomic scale by MD simulations.
- The changes in the morphology of composite coatings and grain sizes, which are consistent with some experimental reports, are made clear by the atomic details.

Abstract

The growth of Al-Graphene composite coatings on polycrystalline Al substrate was investigated by using classical molecular dynamics (MD) simulations. Unlike the diffusion behaviors on single crystal surface, most of adatoms were easily bound by the steps on polycrystalline Al surface, owing to the local accelerated energy. Both Ehrlich-Schwoebel (ES) barriers and the steering effect backed up the volmer-weber growth mode, which was consistent with the dynamic growth process observed in the deposit. The morphology of composite coatings was significantly affected by graphene flakes. Enrichment of graphene flakes gave rise to an increase of the local thickness, and graphene flakes only existed in Al grain boundaries. The size of Al grains in the composite coating visibly decreased when compared with that in the pure Al coating. This grain refinement and the mechanical property can be reinforced by the increase of graphene flakes.

Keywords: MD; graphene; deposition; steering effect; grain refinement

1. Introduction

Metal matrix composite coatings containing nanosized particles used as reinforcement phase have attracted considerable interest in the field of material science and manufacturing, due to the improved mechanical properties. As known to all, the mechanical performances are directly related to the film structure, which is heavily influenced by the evolution of surface morphology

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