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Surface Diffusion and Growth of Alloy Nanoclusters: A Monte Carlo Study

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1. Introduction

Molecular beam epitaxy has become an important tool to prepare ultrathin films and nanostructures in nonequilibrium states that show novel properties distinctly different from the equilibrium bulk phases. Theoretically, the question arises how to relate the structural characteristics of the growing material to the incoming flux and temperature-dependent surface diffusion constants. This question is fairly well understood for one-component systems. By contrast, only few theoretical studies were devoted to the growth of binary alloy nanostructures, despite of the large interest in this field from the experimental and technological viewpoint. In this communication we present detailed kinetic Monte Carlo simulations of growing nanoclusters within a binary alloy model that allows arbitrary diffusion moves of atoms within an active zone near the cluster surface. Our model is designed to describe fcc-type alloys under growth in the (111) direction. The main motivation came from recent experiments on $CoPt_3$ nanoclusters on van der Waals surfaces [1]. Growth-induced structural anisotropy is responsible for a measured perpendicular magnetic anisotropy (PMA), which can be utilized in magnetic storage devices.

2. Simulation method and results

Clusters up to about 3000 atoms are grown by a continuous time kinetic Monte Carlo (KMC) algorithm. Parameters for chemical interactions are chosen in accordance with known properties of $CoPt_3$ crystals. Above room temperature we find facetted clusters and pronounced incubation periods preceding nucleation and lateral growth of a new layer. Such nucleation events on the top layer are largely controlled by diffusion of adatoms along lateral facets, before reaching the upper terrace.

In our analysis we represent the overall structural anisotropy of a cluster by the difference in numbers of Co-Pt bonds parallel and perpendicular to the substrate, $n_{||} - n_{\perp}$. Under the assumption that each Co-Pt bond provides an easy axis for Co-magnetic moments, this quantity should directly reflect the magnetic anisotropy. Negative values of $n_{||} - n_{\perp}$ correspond to PMA. We find that surface segregation of Pt-atoms plays a crucial role in determining that quantity. Pt-surface segregation is driven

by chemical interactions that contribute to the surface field, but is kinetically hindered by the incoming flux. It turns out that additional exchange processes between adatoms with low coordination and atoms in the layer below are crucial to produce significant Pt-segregation. In Fig. 1 we plot $n_{||} - n_{\perp}$ as a function of the number of cluster atoms during deposition. In fact, near room temperature we find negative values consistent with PMA, provided that direct exchange processes described above contribute significantly to the surface kinetics.

3. Magnetic interactions and growth

An influence of the structure on magnetic properties is well established for $CoPt_3$ [2]. Conversely, inclusion of magnetic interactions in our model suggests that application of a magnetic field perpendicular to the substrate should lead to a small increase in the structural anisotropy. The possibility to detect this effect experimentally will be discussed.

4. Conclusions and outlook

KMC-simulations, based on deposition and atomic migration steps, are able to produce structural anisotropies in fcc $CoPt_3$-type nanoclusters which are compatible with the measured PMA. Further issues to be discussed are the influence of an external magnetic field on the growth process as well as the emergence of the ordered $L1_2$-phase through surface diffusion processes under conditions where bulk diffusion is frozen.

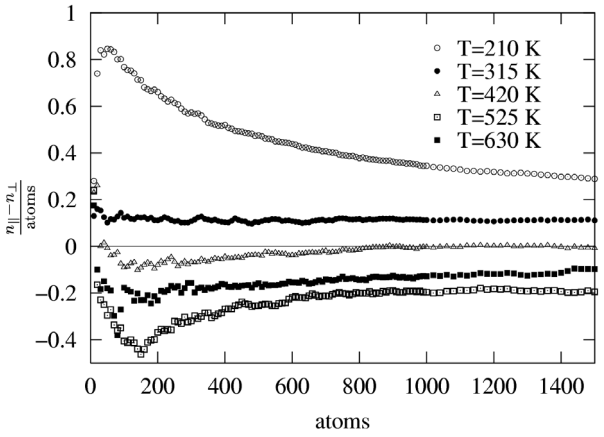

Fig. 1 Anisotropy parameter $n_{||} - n_{\perp}$ as a function of the size of a growing cluster averaged over 10 realizations of the growth process. The mean sampling error at 1000 atoms is about ± 0.03. The simulation also includes exchange processes (see text) with an activation barrier twice as high as the diffusion barrier.

References

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