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Nanostructured Surface of Metals and Alloys Induced by Ar Ion Bombardment

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Self-organized nanostructures of dots, holes or ripples produced by energetic ion bombardment have been reported in a wide variety of substrates. We investigated the atomic scalestructure evolutionoccurringon a pure Pd, $Co_{0.5}Cu_{0.5}$ alloy and the CoAl B2 phase surfaceduring energetic bombardment by Ar. We employed a three-dimensional molecular dynamics (MD) simulation with a combined force field that can consider a large repulsion. It was observed that significant rearrangement of the substrate atoms occurs in a ballistic manner, resulting in the rearranged atoms located higher than the original surface. The lateral distribution of the rearranged atoms has four-fold symmetry along <110> direction on (001) surface. Experimental observation of the four-fold symmetry can be addressed by the lateral distribution of the rearranged atoms. In the alloy system, this bombardment induces a surface composition modulation in layer-by-layer mode. In both the $Co_{0.5}Cu_{0.5}$ alloy and the CoAl B2 phase, the element of higher-sputtering yield is accumulated on the top surface layer, whereas it is depleted in lower layers. A kinetic model considering both the rearrangement and the sputtering of the substrate atoms agrees with the puzzling simulation results, which revealed that the rearrangement of the substrate atoms plays a significant role in the observed composition modulation.

Keywords
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