SF-P020

Layer-by-layer Composition Modulation by Ion-induced Atomic Rearrangement in Metallic Alloys

김병현[1,2], 김상필[1,3], 이광렬[1], 정용재[2]

[1]한국과학기술연구원 계산과학센터, [2]한양대학교 신소재공학과,
[3]Brown University, Division of Engineering

Self-organized nanostructures of dots, holes or ripples produced by energetic ion bombardment have been reported in a wide variety of substrates. Ion bombardment on an alloy or compound also draws much attention because it can induce a surface composition modulation with a topographical surface structure evolution. V. B. Shenoy et al. further suggested that, in the case of alloy surfaces, the differences in the sputtering yields and surface diffusivities of the alloy components will lead to a lateral surface composition modulation [1]. In the present work, the classical molecular dynamics simulation of Ar bombardment on metallic alloys at room temperature revealed that 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.

References

V. B. Shenoy, W. L. Chan and E. Chason, *Phys. Rev. Lett.* **98**, 256101 (2007)