Growth, strain, and stability of metal and oxide thin films

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論 文 内 容 の 要 旨
Thesis Summary

Strains in metal and oxide thin films, which comes from lattice mismatch with the substrate lattice, results in unique crystal structures and chemical reactivity. Novel two-dimensional materials derived from these distortions have been explored and their physical properties have been investigated. In this thesis, the growth, structure, and electronic properties of thin tin films on molybdenum and tungsten surfaces and iron and iron oxide on ruthenium surfaces are mainly revealed using low energy electron diffraction and ab-initio DFT calculations.

In Chapter 1, the background of this study is outlined. The crystal structures, electronic structures, and chemical reactivity of tin, iron, and iron oxide thin films grown on metal surfaces are described.

Chapter 2 describes principles of crystal structures, thin film growth, and gas adsorption in solid surface science.

Chapter 3 describes the properties of the elements used in this study and experimental techniques such as slow electron diffraction and molecular beam epitaxy.

Chapter 4 describes tin thin films on molybdenum(110) and tungsten(110). Since both molybdenum and tungsten have a body-centered cubic structure and the difference in lattice constants is only 0.8%, it is known that thin films on molybdenum and tungsten surfaces have similar structures. As the coverage of tin increases on molybdenum(110), the Sn films exhibit 3x1, 1x3, and 1x4 structures, where 1x3 is considered as an elongated β-tin structure and 1x4 as a tin monolayer structure very close to β-tin. The 3x1 structure with the lowest coverage is found to be a tin-molybdenum surface alloy. On the other hand, tin thin films on tungsten(110) show 1x3 and 1x4 structures with increasing tin coverage, similar to molybdenum, but the 3x1 surface alloy structure does not appear even at high temperatures. Furthermore, the 1x3 structure is newly found to undergo a temperature-reversible phase transition below a room temperature. This finding indicates that the tin-tungsten interface is very stable and that tin on tungsten is useful as a new two-dimensional material.

Chapter 5 describes iron films on ruthenium surfaces and their initial oxidation processes. The structure of the iron film on the ruthenium surface is strained by +6.3% compared to that of the bulk. The structure of this strained iron film is determined with high precision by low electron energy diffraction. In the initial oxidation process from metallic iron to iron oxide, it is experimentally shown that the p(2x2) and c(4x2) superstructures coexist at room temperature with an oxygen coverage of 0.25. First-principles DFT calculation reveals that the energies of the p(2x2) and c(4x2) superstructures are very similar. The adsorbed oxygen on the strained iron film is also close to the substrate ruthenium with a high coordination number and the adsorption structure is particularly stable at low oxygen coverage.

Chapter 6 summarizes all the findings of this study and gives general conclusions.