Atomic Level Characterization of Initial Oxidation of Si and SiC and of Initial Reactions at Ni/Si and Ni/SiC Interfaces

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I have studied the initial reactions of oxygen and nickel with clean Si and SiC surfaces by high-resolution medium energy ion scattering (MEIS) and synchrotron-radiation-light induced photoelectron spectroscopy (SR-PES).

First, probable structure models are proposed for the oxidized Si(111)-7×7 and Si(001)-2×1 surfaces at room temperature(RT). It is revealed that the oxidation of the Si(111) surface at high temperatures proceeds in a layer-by-layer fashion and in contrast the Si(001) surface is oxidized non-uniformly. For the oxidation of the 6H-SiC(0001)-$\sqrt{3}\times\sqrt{3}$ surface at RT, the adatoms giving a $\sqrt{3}\times\sqrt{3}$ periodicity are preferentially oxidized and it leads to formation of Si^{3+} and Si^{4+} states. No uniform SiO2 layer is formed on the (0001) surface even at a high temperature of 700°C. I have also analyzed structure and oxidation of the 6H-SiC($11\bar{2}0$) surface and clarified its atomic and electronic structures for the first time. The MEIS analysis reveals the existence of a Si-adlayer of 0.5 ML (1 ML = 1.49×10^{15} atoms/cm^2) on the ($11\bar{2}0$) surface, which is predicted by a recent first principle density functional theory. The Si-2p and C-1s core level analysis supports the existence of the above Si-adlayer. The MEIS and SR-PES analyses indicate that two oxygen atoms are inserted side by side into the corner bridge-site between two corner adatoms and the backbond connected the 2nd-layer Si atom. It as also shown that uniform ultra-thin SiO2 layers with abrupt interfaces are formed by thermal oxidation at temperatures higher than 500°C. Furthermore, a compressive strain of 2 % in the surface normal direction is detected for the SiC($11\bar{2}0$) substrate just below the interface using the ion shadowing effect. Finally, the initial reactions of Ni with the Si(111) and 6H-SiC(0001) surfaces have been analyzed *in situ* by reflection high energy electron diffraction (RHEED), MEIS and SR-PES and *ex situ* by atomic force microscope (AFM).

This work covers wide fields of the initial reactions of oxygen and metal atoms with the clean Si and SiC surfaces and of the structure of the interfaces. I believe that the present study would contribute to understanding the fundamental surface physics and chemistry and also to industrial device fabrications.