博士論文を要約したもの

博士論文題目

Scanning tunneling microscopy study of various Si surfaces interacted with Fe atoms and gas molecules

（清浄および Fe 原子や気体分子と相互作用した Si 表面の走査トンネル顕微鏡研究）

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（要約）

Using non-equivalent status of material surfaces, various functional metastable materials can be synthesized by metal deposition and molecule adsorption. The abrupt interactions lead to separated quasi two-dimensional deposited materials, while mixed interfaces lead to compound materials with different properties. The creation of these interfaces utilizing metal, molecule and substrate interactions is one of key techniques for materials construction.

This dissertation studies four types of interacted systems. The interactions are between surface and molecules (interaction 1), between surface and metals (interaction 2), between surface compound with molecules, and metals (interaction 3), and between surface compound with metals, and molecules (interaction 4). The dissertation focused material systems related to Fe metals and Si substrates with some kinds of molecules, mainly based on Fe-silicide compounds formation which shows the wide range properties in various phases. The study of fabricated Si(110) side-surfaces after the molecular etching process is to extend the two-dimensional substrates to three-dimensional substrates for next stages of molecular adsorption and iron silicide formation. These topics are described in chapters 2-6. All the surface systems are studied by scanning tunneling microscopy (STM) at room temperature in ultra-high vacuum at atomic scale.

Chapter 2 (interaction 3). The investigations of initial adsorption of Fe on ethanol-saturated Si(111)7×7 surface by using the newly statistical analysis of adatom height histogram in STM images revealed the protection of the molecule termination at adatoms from the Fe capturing at the initial stage. Fe reaction rate at bare center-adatoms was higher than that at bare corner-adatoms at the initial stage. The analysis also suggested to discriminate molecules with the large rotation freedom.

Chapter 3 (interaction 1). NO adsorption on Si(001)2×1 surfaces at the same area in STM indicated multiple configuration types firstly, which were compared to models in the previous density functional theory (DFT) calculations, with residual H_2O adsorption. The ordering on the surface was destroyed after large amount exposure.

Chapter 4 (interaction 2). In the formation of β-$FeSi_2$(100) on Si(001), two types defects were found in further annealing. According to DFT calculations, bright pair-defects were suggested to be two adjacent Si-vacancy, while the dark single-defects were probably caused by Si_4-vacancy.

Chapter 5 (interaction 4). Molecules adsorption on β-$FeSi_2$(100)/Si(001) surfaces were studied with air, poor vacuum, NO and atomic-H. In this study, lower reactivity of β-$FeSi_2$ than

that of Si(001) was found. The atomic-H adsorption was hard to be observed by STM as predicted by DFT, but the existence of hydrogen on surface or in bulk was demonstrated by H_2 thermal desorption. It was noted that atomic-H could not reduce the surface states near Fermi levels in the band gap of β-$FeSi_2$.

Chapter 6. Side-surface of artificial substrate structure in a three-dimensional Si{111} vertical side-surface structure on a Si(110) wafer was fabricated by reactive ion etching. STM successfully displayed an atomically-flat 7×7-reconstruction on the side surfaces.

In summary, the dissertation revealed some key properties in molecules and/or Fe-metals behavior on Si substrates using atomically resolved STM: ethoxy molecules preventing Fe atoms toward extreme molecular mask, initial adsorption stage of nitric oxide on Si(001) leading to SiON materials, defect formation on β-$FeSi_2$ surfaces which will perturb electric conductivity, molecule-modified β-$FeSi_2$ surfaces toward surface-property control. The successful construction of atomically flat side-surfaces will promise highly integrated circuits using the molecules, metals and substrates interactions, in next generation.