Atomic Structure of the Si(553)-Au Surface at Room Temperature and Low Temperature

When gold atoms are deposited onto the (553) surface of silicon, one-dimensional structures can be formed. In this work, the atomic structure of these one-dimensional structures and the structural changes occurring in a metal-insulator transition on the surface were investigated with surface X-ray diffraction. It was found that the gold atoms form chains along the steps on the surface, while the silicon atoms near the step edges reconstruct to a graphite-like structure. In the metal-insulator transition the gold atoms and nearby silicon atoms form a doubled periodicity along the steps. The changes in the diffracted intensity with temperature below the phase transition temperature are consistent with a Peierls transition.

Materials with one-dimensional electronic states have properties that can be strikingly different from those in three dimensions, because of the confinement of the electrons and their strong correlation. An example for a phenomenon that can occur in one-dimensional systems is a phase transition from a high-temperature metallic state to a low-temperature insulating one, involving the formation of periodic charge density waves and corresponding lattice distortions (Peierls transition).

One possibility to make one-dimensional structures is by depositing small amounts of gold atoms onto stepped silicon surfaces [1], for example onto the (553) surface (denoted Si(553)-Au). This surface is composed of terraces with a 111 orientation separated by steps one atomic layer high. Gold atoms deposited onto this surface form one-dimensional structures parallel to the steps. They are especially interesting because they are metallic above room temperature, but at lower temperatures two phase transitions occur just above room temperature and at about 250 K, in which they become insulating [2].

In this research, the atomic structure of the Si(553)-Au surface and the structural changes in the metal-insulator phase transition near room temperature were investigated with surface X-ray diffraction. Experiments were done *in-situ* in ultra-high vacuum with the six-circle diffractometer at BL-15B2. X-ray diffraction intensities from crystal truncation rods were collected at room temperature for the structural determination. The structural changes in the phase transition near room temperature were investigated by measuring at 86 K diffraction intensities from the superstructure developing below the transition. The temperature dependence of diffraction profiles from the superstructure was measured between 86 K and 770 K.

The determination of the surface structure was done using Patterson analysis [3]. The Patterson map is calculated by Fourier-transforming the measured diffraction intensities (Fig. 1). Peaks in the Patterson map correspond to vectors between atoms in the structure. The structural model extracted from the Patterson map is shown in Fig. 2. The gold atoms align parallel to the step edge. The structure of the silicon atoms is different from that of a bulk-terminated surface, they form a honey-comb chain structure with a graphite-like bonding configuration near the step edge.

An uncertainty in the determination of the structure is the amount of gold on the surface. Most published reports assume one gold chain per step, but a recent investigation showed that two gold chains per step are more likely [4]. In the latter case, the model in Fig. 2 can be modified by replacing the silicon atom immediately right of the gold atom with another gold atom. This also improves the reproduction of the Patterson map at the strong peak at x=0.08, z=0.03.

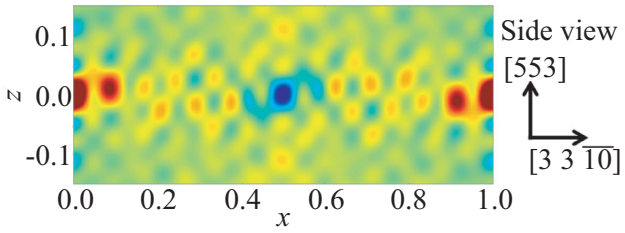

Figure 1
Patterson map calculated from the X-ray diffraction intensities from the Si(553)-Au surface. Red/orange peaks correspond to vectors between atoms. x and z are in fractions of the unit cell.

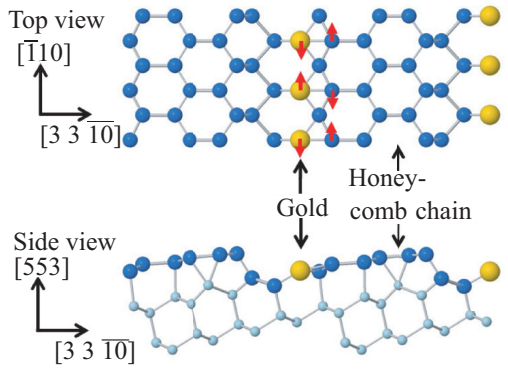

Figure 2
Structural model for the Si(553)-Au surface. The red arrows indicate possible displacements in the metal-insulator transition.

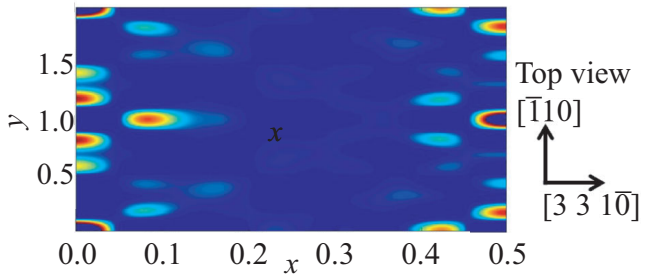

Figure 3
Patterson map calculated from the low-temperature superstructure intensities. Red/yellow peaks correspond to vectors between atoms participating in the formation of the superstructure. x and y are in fractions of the unit cell.

At temperatures below the metal-insulator transition the periodicity along the steps doubles to form a superstructure. The structural changes responsible for the formation of the superstructure were investigated by measuring the diffraction intensities originating from the superstructure [5]. It contains only information about the atoms involved in the superstructure. The Patterson map calculated from these intensities is quite simple and shows that only a few atoms are involved in the superstructure (Fig. 3). The dependence of the diffracted intensity from the superstructure on the X-ray wavelength near the L_{III} absorption edge of gold shows that the gold atoms are participating in the superstructure. An example of possible displacements of the atoms at low temperatures is indicated by the red arrows in Fig. 2.

The mechanism responsible for the phase transition can be investigated by measuring the temperature dependence of the profile of a reflection. The results are consistent with the predictions by mean-field theory for a Peierls transition [5].

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