Surface Structure of Initial Ag Deposition on Si(100) and Its Local Density of State

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Abstract

We investigated the initial stage of Ag adsorption on Si(100) surface at low temperature. We observed another adsorption structure at low temperature in comparison with room temperature. We also measured the I-V characteristic over Ag sites which indicate two distinct peaks of negative differential resistance in the empty state. The mechanism behind this phenomenon is attributed to the localized surface states of Ag within the Si bulk band gap.

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1. Introduction

There are many studies of metal on semiconductor surface which are related with physical interest and industrial applications. With developing of surface analysis techniques, the objectives have been extended to various directions. Now we can make various states of many kinds of metal, for example thin film, clusters and atoms.

Now many groups are trying to make nano-structures by self assemble, lithography, STM techniques and so on. One of our objectives is studying these structure and their density of state. In this paper, we report the initial stage of Ag on Si(100). A different adsorption model is proposed based on our STM results. Most significantly, we present the I-V data over isolated Ag features which exhibit the negative differential resistance(NDR)[1] in the empty state.

2. Experimental

Sample preparation and measurements were performed in a JEOL JSTM-4500XT system composed of preparation chamber and an STM camber. Si(100) specimens($1.0\times6.5\times0.38$ mm^3) were cut from commercial polished Si wafer (n-type, $\sim0.005\,\Omega$cm).Atomically flat Si(100)2×1 surfaces were obtained after outgassing the sample at ~400℃ for ten hours and flashing up to ~1200℃. The sample was cooled down via a cryostat which is mounted in the STM chamber and was filled with liquid nitrogen in the present experiment. (The liquid nitrogen in the cryostat was blown away before making any measurements in order to avoid vibration due to bubbling.) After the temperature of the sample holder had stabilized at ~80K, the sample was transferred to the preparation chamber for subsequent metal deposition. As results of the residual cooling of the sample holder, the substrate temperature is expected to be much lower than room temperature during deposition. Silver metal was evaporated from a tungsten basket at a base pressure $< 10^{-7}$ Pa with a coverage of 0.05 ML estimated by counting Ag features observed in the STM images(1 ML= 6.8×10^{14} atoms/cm^2).Imaging and tunneling spectroscopic measurements carried out in the STM chamber at ~200K with background pressure of 2×10^{-8} Pa. All images were taken in the constant current topographic mode with the sample biased(i.e., tip-ground).

3. Results and discussion

Fig.1 shows dual-bias images(25 nm$\times$18 nm, 3 nA) of Ag on Si(100) for a 0.05 ML coverage with tunneling into and out of the same area at bias voltages of (a) -1 V(occupied state) and (b) +1V(unoccupied state). The images were simultaneously acquired at 195K in which the forward scan corresponds to one type of polarity while the backward scan to the opposite. Sometimes a shape of tip apex affects STM images[2,3], by taking STM images with this method we can get them in same tip apex condition. Since the difference of images at each voltage is clearly caused by electronic state at each voltage. In order to discern the adsorption geometry, magnified images of a typical region from Fig. 1 (a) and (b) are shown in Fig. 1 (c) and (d), respectively. The corrugation profile over a bright Ag feature along the Si dimer row direction is given in

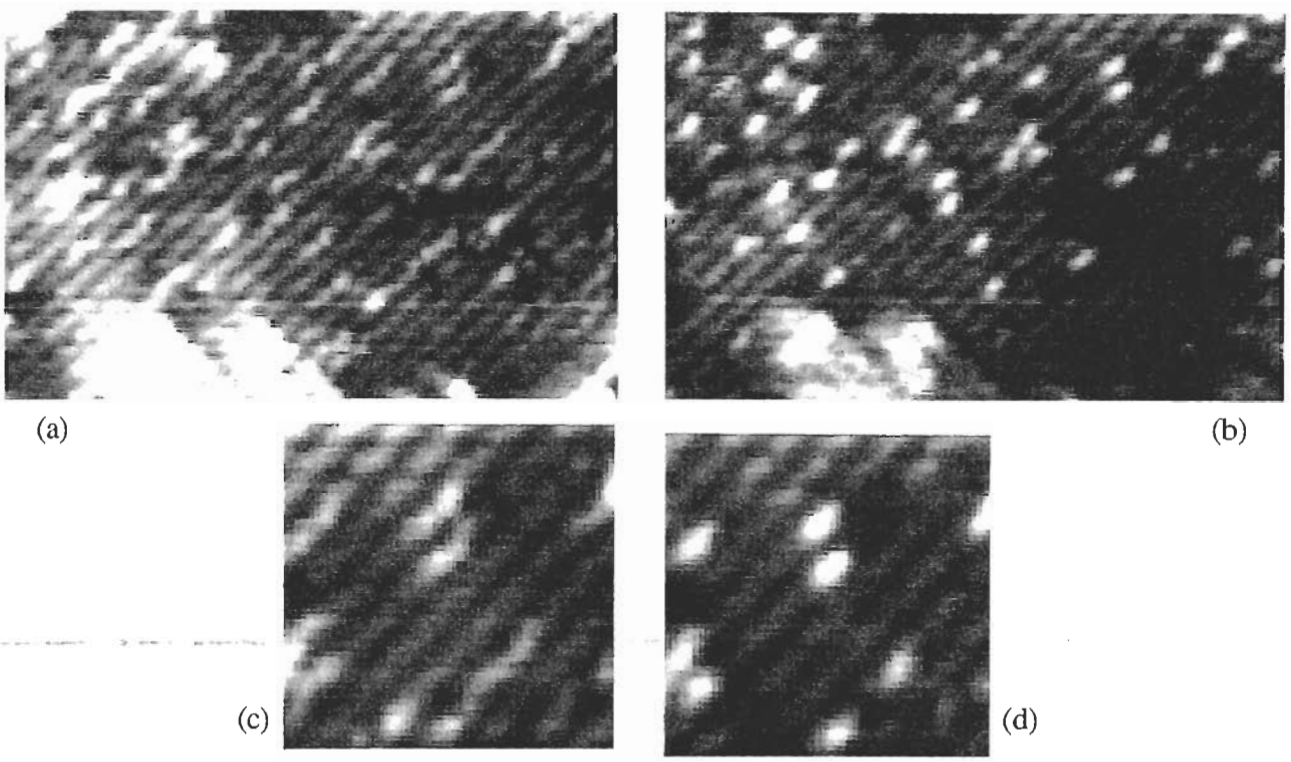

Fig.1 STM images(25 nm×18 nm, 3 nA) over the same area of Si(100) covered with 0.05 ML Ag at 195K. (a) -1 V, occupied state, (b) +1 V, unoccupied state, (c) and (d) are zoom-in images from (a) and (b) respectively.

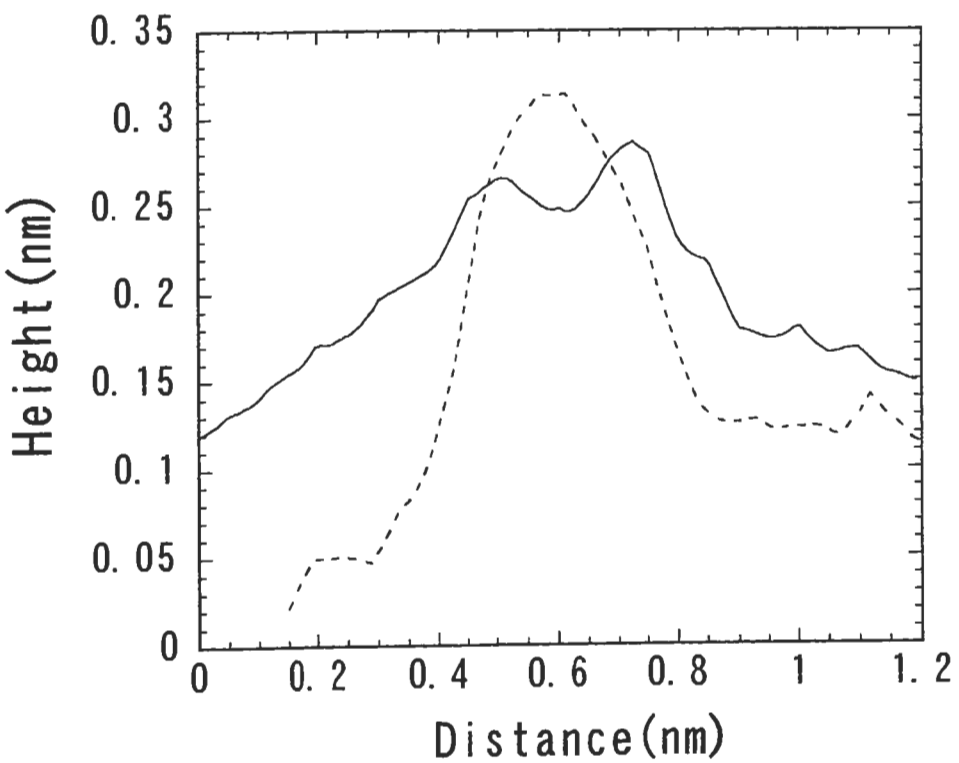

Fig.2 The curves mean topographical height around Ag site along Si dimer-row from Fig.1. The solid and the dotted line are got from -1 V and +1 V respectively.

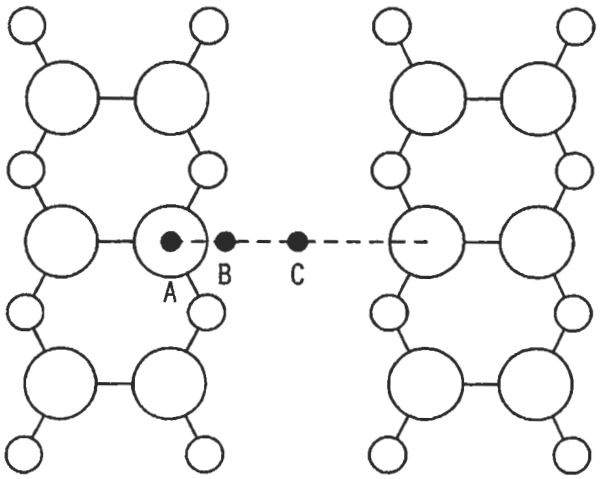

Fig.3 Schematic diagram of Ag adsorption on Si(100).The black and white circles represent Ag and Si atoms respectively. A, B and C mark possible positions for Ag adsorption on Si(100).

Fig.2. These data suggest that the bright protrusion corresponds two Ag atoms, with the feature best seen in the occupied state image in conjunction with the corresponding topographic height analysis, in which two separate Ag atoms are resolved with a spacing of~3.8Å. Generally STM images represent equipotential surface of electrons, more precisely speaking, integration of density of state from Fermi energy to bias energy. So the orbital at occupied state behaves like anti-bonding and the one at unoccupied state like bonding.

We show models of adsorption structure in this experiment in Fig.3. From Fig.1 adsorption structure looks (A) or (B) in Fig.3. But this result is different from other groups' experimental results of Ag/Si(100) at room temperature[4]. They indicated that the position of Ag adsorption is (C) in Fig.3. Especially Samsavar et al. said that Ag could be in a valence-2 state. In way of comparison STM images of alkali metal on Si(100)[5,6] are similar to our results. Ag([Kr](4d)^{10}(5s)^{1}) belongs IB group and is transition metal. In our low temperature experiment Ag behaves in a valence-1 state.

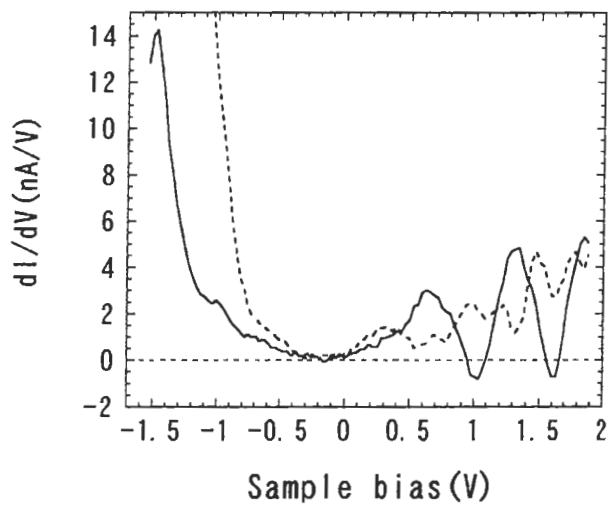

Fig.4 Tunneling spectroscopy at 195K on the Ag/Si(100) over a Ag site(solid) and a Si-dimer site(dotted).

Fig.4 shows tunneling spectroscopy at 195K. There are two NDR(+1.0V and +1.6V) states on Ag site. But these peak positions and the quantities are not always same. Because the shape of the tip apex is not always same, the electronic state of the tip is changed. The electronic state of the tip apex is not able to be neglected. The tunneling current depend on transition between the density of state of the tip and the one of the sample. I.-W.Lyo et al. simulated NDR to use easy model[7]. They supposed that both density of states of a tip and a sample were localized. As mechanism of tunnel diode, when electron throw at the interface of p- and n-type semiconductors, NDR appears by the relation energy gaps and Fermi energies. Since NDR is caused by varied energy distribution of density of states. We took NDR on Ag sites, so we think that surface state presents locally in energy gap of Si bulk by Ag adsorption on Si(100).

4. Conclusion

We observed at about 200K the surface of Si(100) on which Ag was deposited at low temperature(80K < T << room temperature). From STM images at -1V and +1V, occupied and unoccupied orbital of neighboring two Ag sites are uncoupled and coupled respectively. In comparison with another experiment at room temperature[4] there are another adsorption structure of low coverage Ag on Si(100) by deposition at low temperature. Ag adsorbed on Si(100) as valence-1 at low temperature. We observed NDR of tunneling spectroscopy on Ag site. We think that there are local surface state in Si bulk gap.

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