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Electrical conductance at initial stage in epitaxial growth of Pb, Ag, Au and In on modified Si(1 1 1) surface

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Abstract

The electronic properties of thin metallic films of Pb, Ag, Au and In atoms deposited at 105 K on well defined metallic surface, i.e. Si(1 1 1)-(6 × 6)Au surface with 10 ML of annealed Pb, were investigated using four-point probe method in UHV condition. The structure of the substrate and deposited metals were monitored by the RHEED system. The electrical conductance, measured during the deposition of In and Pb atoms, shows the local minimum for the coverage equals about 0.3 ML whereas for Au and Ag atoms the conductance decreases during the first monolayer growth. For Au atoms the local maximum in the conductance was observed for the coverage about 0.55 ML, which can be connected with localized states. To describe theoretically the conductance behavior the tight-binding Hamiltonian and equation of motion for the Green's function were used and good qualitative agreement was obtained.

Keywords: Epitaxy; Electron diffraction; Conductance; Tight-binding model; Green's function

1. Introduction

Recently, there has been considerable progress in fabrication and theoretical analysis of two-dimensional (2D) electron systems, e.g. [1]. Especially interesting are very thin atomic layers (metallic, semiconducting or ferromagnetic) disturbed by other atoms. In particular, a distribution of such atoms on a surface is a quantity of great interest because it determines the electrical conductance through the system and can regulate the flow of current. It is known that 2D conductance strongly depends on the surface scattering centers and thus even very low number of atoms on a surface can blockade the current. Due to this reason such 2D systems can be considered as a potential candidate to fabricate (or improve) different kind of nanodevices, e.g. smaller and faster nanotransistors, logic gates etc. Moreover, a stripe of metallic film can be considered as a perfect and stable electric wire which can connect two nanodevices (monoatomic quantum wire is the thinnest possible conducting wire, but is very sensitive on external conditions and can be easily broken). It is very important to know how the current flowing through such a metallic film is modified in the case when other atoms are situated on it. Therefore the experimental studies must concentrate on very low coverage regime i.e. thin metallic film should be covered by submonolayer amount of different atoms (adatoms).

Most studies of the electrical conductance of well ordered surface with deposited unreactive metals have been conducted on clean or reconstructed substrates for the coverage higher than 1 ML. Hasegawa and Ino monitored the conductance dependence on the surface structures and epitaxial growth modes at initial stage of Ag and Au deposition on Si(1 1 1) surface at room temperature [2]. Takeda et al. have characterized the changes in surface electrical conductance induced by additional indium deposition onto clean and reconstructed Si(1 1 1)-7 × 7 surfaces [3]. Recently Yamazaki et al. have succeeded in detecting the electrical conductance on different Si(1 1 1)/Au surface superstructures using micro-four-point methods [4]. In our previous investigation [5] it was shown the strong influence of used

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substrates on the behavior of the conductance during the epitaxy of Pb atoms on Si(1 1 1)-(6 × 6)Au surface which was modified by the very low amount of annealed Pb atoms (with up to 4.2 ML). There are three parallel channels for electrons which flow through such structures: (i) the top most atomic layers with surface-states, (ii) surface-space-charge layer and (iii) unperturbed bulk crystal. A number of attempts were reported for measuring and estimation of the conductivity through different channels [6,7]. On the other hand our previous studies [5], were limited to a low Pb coverage regime, where magic islands can be most abundant. Although those issues have been addressed, resent studies show that preparation an atomically flat metal films on semiconductor substrate remains a great challenge. A low temperature deposition of Pb on modified Si(1 1 1) surface and slight annealing (up to room temperature) method could fulfill those requirements. Recent extensive investigations have been made for studying an intriguing thickness and thermal-dependent stabilities of Pb layers [8–12]. These investigations suggest that below the critical thickness of 10 ML of Pb all flat films formed at low temperatures are unstable. Above 10 ML Pb films become stable even at room temperature.

In this paper, we focus on the measurements of the electrical conductance at initial stage in epitaxial growth of Pb, Ag, Au and In on Si(1 1 1)-(6 × 6)Au/Pb (i.e. Si(1 1 1)-(6 × 6)Au with 10 ML of annealed Pb) surface using four-point probe method. We have chosen Si(1 1 1)-(6 × 6)Au surface as a base one because during the deposition process it guarantees the layer-by-layer growth almost from the beginning of epitaxy (Si(1 1 1)-7 × 7 reconstruction fails in this regime of deposition). Moreover, we use 10 ML of Pb on Si(1 1 1)-(6 × 6)Au surface to avoid the magic islands growth and also to fabricate rather flat, metallic substrate with very limited number of surface scattering centers (to make the substrate better it was annealed up to room temperature). After recrystallization of 10 ML Pb the surface scattering should be less important. Presence on this metallic surface new Pb, Ag, Au or In individual atoms increases the roughness and therefore a diffuse scattering of electrons at the surface.

Electrical properties of thin metallic films disturbed by deposited atoms have been investigated theoretically by many authors. The most popular theory is a microscopic quantum-mechanical description, e.g. [13], which include both the surface and bulk scattering and was successfully used to describe quantum size effect in Pb and Pb/In films [14]. Also the influence of surface roughness on the conductivity of 2D atomic system was investigated using the theory based on Boltzmann-like equation with an autocorrelation function associated with the surface roughness [15]. Effects of rough boundaries on density of states and conductance through one-dimensional and quasi-two-dimensional channels were studied using Green function method [16,17]. Electron scattering effects by random surface corrugation were considered in Ref. [18] (short review article) using surface correlation functions. The Born approximation [19,20], diagrammatic technique [21], Kubo formula [22] or density matrix method [23] can be also used to describe the conductance of thin metallic or semiconductor film. Recently ab initio methods using the density functional theory have been applied to analyze the transport properties of ultrathin films, e.g. [24]. The most studies in this field concentrate on rather thick coverage regime (above 1 ML). Neither of mentioned above papers have analyzed the conductance of thin metallic film with additional atoms on it in the low coverage regime, i.e. the processes which take place where submonolayer coverage of the film is considered and single or small cluster of atoms exist on the surface. Depending on the kind of additional atoms and surface material most of the cited above theories break down in this regime.

In this paper, the experimental results are analyzed using the theoretical model based on the Green's function method and thigh-binding Hamiltonian. The model allows us to calculate the electrical conductance of 2D lattice of atoms connected with a metallic surface and with two electrodes. On such atomic lattice single atoms are deposited and they disturb the current flowing through the system. This model simulates the initial stage of growth observed during the deposition process and can be useful to explain the conductance behavior in our experiment. In comparison with other theories the model we consider here can describe the conductance for different crystalline structure of the surface, for different distribution of external atoms on a surface and due to the parameters of the system (like electron energies, hopping integrals) can distinguish between different kind of coupled atoms. Moreover, this formalism do not use the continual value of the layer thickness parameter. For the very initial growth a thickness parameter cannot be treated as the effective one but the thickness should be obtained on the basis of the relative proportion between the number of additional atoms and surface atoms.

The paper is organized as follows. The description of the experiment and the results concerning the conductance changes during the deposition of Au, Ag, In and Pb atoms as well as the temperature changes of the conductance are included in Section 2. Moreover, in this section the reflection high energy electron diffraction (RHEED) pictures for different atom distributions are shown. Section 3 provides a quantum description of the conductance. The theoretical model and calculation method are presented in Section 3.1. The numerical calculations of the conductance and comparison with the experiment are included in Section 3.2. The results are discussed in Section 4. Section 5 is devoted to conclusions and in Appendix A we calculate the conductance for analytically solvable simple cases which can be helpful to understand how our theoretical model works.

2. Experimental setup and results

The measurements were performed in a UHV chamber with a base pressure in order of 5×10^{-11} torr. The