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ScienceDirect

Surface Science 601 (2007) 5403–5411

SURFACE SCIENCE

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Electron and lattice structure of ultra thin Ag films on Si(1 1 1) and Si(0 0 1)

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Received 15 June 2007; accepted for publication 3 September 2007
Available online 20 September 2007

Abstract

We studied the low temperature ($T \leqslant 130$ K) growth of Ag on Si(0 0 1) and Si(1 1 1) flat surfaces prepared by Si homo epitaxy with the aim to achieve thin metallic films. The band structure and morphology of the Ag overlayers have been investigated by means of XPS, UPS, LEED, STM and STS. Surprisingly a $(\sqrt{3}\times\sqrt{3})$R30° LEED structure for Ag films has been observed after deposition of 2–6 ML Ag onto a Si(1 1 1)$(\sqrt{3}\times\sqrt{3})$R30°Ag surface at low temperatures. XPS investigations showed that these films are solid, and UPS measurements indicate that they are metallic. However, after closer STM studies we found that these films consists of sharp Ag islands and $(\sqrt{3}\times\sqrt{3})$R30°Ag flat terraces in between. On Si(0 0 1) the low-temperature deposition yields an epitaxial growth of Ag on clean Si(0 0 1)-2×1 with a twinned Ag(1 1 1) structure at coverage's as low as 10 ML. Furthermore the conductivity of few monolayer Ag films on Si(1 0 0) surfaces has been studied as a function of temperature (40–300 K).

Keywords: Low energy electron diffraction (LEED); Visible and ultraviolet photoelectron spectroscopy; Scanning tunneling microscopy; Scanning tunneling spectroscopy; Surface relaxation and reconstruction; Surface electrical transport (surface conductivity, surface recombination, etc.); Silicon; Silver

1. Introduction

Most semiconductor surfaces reconstruct after metal deposition onto clean surfaces which is subject of many investigations. In particular, the Ag/Si(1 1 1) and Ag/Si(0 0 1) surfaces have been studied by almost every surface analysis techniques and many different surface phases (SP) have been observed for monolayer and sub- monolayer coverage's (see [1–24] and references therein). At larger coverage's however, the metals are known to form 3D-cluster structures at RT due to the large lattice mismatch with respect to Si substrate. In general the metal lattice parameter is smaller than those of the semiconductors. The hetero epitaxial growth of the metal films on semiconductors is a topic of great fundamental and technological interest [1,2], in particular due to its potential in the development of quantum devices.

Recently, a breakthrough has been achieved in this field by use of low substrate temperatures during the growth of metallic films [2–12]. The high mobility of metal atoms at RT is tremendously diminished at low temperatures which overcomes the tendency toward islanding. In fact, the layer-by-layer growth of Au as well as Ag films on Si(1 1 1) at 95 K was concluded as evidenced by RHEED intensities oscillations as a function of coverage [10–12]. This 2D growth mode of Ag on Si(1 1 1) at low temperatures has been confirmed by low-temperature STM investigations [3]. However, small 2D Ag islands (20–40 Å size at 4–5 ML coverage) rather than continuous films have been observed. Interestingly a layer-by-layer growth of Pb films at low temperatures was evidenced by RHEED oscillations when the Si(1 1 1)7×7 substrate was modified by submonolayer Au deposits (Si(1 1 1)$\sqrt{3}\times\sqrt{3}$Au or (6×6)Au structures) prior to the Pb deposition [11,12]. Similar

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0039-6028/$ - see front matter © 2007 Published by Elsevier B.V.
doi:10.1016/j.susc.2007.09.020

results have been obtained for Au and Ag growth on Si(111)$\sqrt{3}\times\sqrt{3}$Ag (hereafter $\sqrt{3}$Ag/Si) and Si(111)$\sqrt{3}\times\sqrt{3}$Au substrates, respectively [13,14]. It was concluded that the epitaxial growth of these noble metals is promoted by the formation of a 2D Ag wetting layer on the Si(111) surface. Furthermore, the continuous growth of Ag(111) films on Si(001) at low temperatures has been observed by SPA-LEED oscillations and STM investigations [4–9]. It is reported that the electrons are confined in metallic islands due to the lack of translational symmetry thus producing quantum well states (QWS) [15–18]. These states begin to appear as the thickness of a 2D layer becomes comparable to the de Broglie wavelength of electrons and have been observed by photoemission studies [15–18].

Despite the wealth of obtained information, the details of the electron structure of $\sqrt{3}$Ag/Si SP are still controversial. In fact, recently it was shown that this superstructure exhibits an isotropic and parabolic surface state band crossing the Fermi level, which gives rise to a 2D metallic like system [2,19]. The electrical conductivity of a Si(111)7×7 and $\sqrt{3}$Ag/Si surface was measured in UHV by a microscopic four-point probe method [20]. Clear evidence of an unusual two order of magnitude enhancement of surface conductivity by deposition of 1 ML $\sqrt{3}$Ag/Si SP and reducing the probe space from millimeter scale to the micron one was obtained. Even though some experimental evidence of electrical conduction through $\sqrt{3}$Si/Ag SP band by aid of four-point microprobe millimeter and micrometer scale experiments at room temperature has been described [2], this result is in contrast to the observation of nonmetallic behavior of $\sqrt{3}$Ag/Si SP at low temperature measurements [4,5]. The disadvantage of these conductivity experiments performed at room temperatures is that the surface conductance is screened by the substrate. Therefore low temperature experiments are crucial for an ambiguous conclusion.

In our group several studies of conductance and structural properties of metal films (Cr, In, Pb) on semiconductor surfaces have been performed. We reported on the growth and the *ex-situ* temperature dependence of the electrical conductivity and the magnetoresistance tensor components of the Si(111)–Cr($\sqrt{3}\times\sqrt{3}$)R30°, Si–In(1×1)R30° surface phase and of ultrathin Si–Cr films covered by a thin amorphous αSi protecting layer [21,22]. We found that Si–In-αSi SP is a 2D semiconductor with an enhanced mobility, while Si–Cr-αSi SP behaves metallic with a rather low mobility. Lately, the *in situ* temperature dependence of conductivity of the Si(111)-7×7 and SP of In and Pb on clean Si(111) surfaces prepared at room temperature have been studied [23,24]. It was shown that both Si–Pb-αS and Si–In-αSi SP exhibit semiconductor 2D behavior with a very small mini gap (0.09 meV and 0.0035 meV, respectively). The percolation behavior and metal–insulator transition was observed for In [23] and Pb [24] island films on Si(111).

Recent experiments [2,4,5] show that 2D conductivity may be realized in Ag superstructures on Si. The measurements of the resistivity of epitaxial metal films are very important for the study of an ideal 2D metallic system. Unfortunately, these studies of conductivity were performed on samples with no *in situ* control of the surface structure, such as STM. Amorphous and granular films may show rather peculiar effects like a change of the sign of temperature coefficients of the resistance. Therefore, we performed new experiments for LT deposition of Ag films and LT conductivity measurements combined with electron structure and morphology investigations of these films.

In this paper we describe XPS, UPS, LEED, STM and STS as well as the electron transport measurements that show very peculiar properties of Ag superstructures on Si(111)7×7 and Si(100)2×1 atomically flat surfaces prepared by homo epitaxy. The low temperature growth of Ag thin films on preliminary prepared $\sqrt{3}$Ag/Si SP results in epitaxial metallic films on Si(111) substrates according to XPS, UPS and LEED studies. However, STM investigations indicate sharp Ag island formation with $\sqrt{3}$Ag/Si layers in between. For the Si(100)/Ag case, we observe 2D-LT growth of continuous metallic flat Ag(111) films. A remarkably high conductivity for these films is found which decreases as a function of temperature between 100 K and 45 K, where the substrate becomes almost insulating. By using well prepared substrates at low temperatures we were able to measure almost pure surface state conductance even over macroscopic distances.

2. Experimental

The growth experiments have been performed in an UHV multichamber surface analytical system with a base pressure of 2×10^{-8} Pa, which allows *in situ* preparation of the Si surfaces as well as characterization by means of ARUPS, XPS, AES, LEED and STM [25,26]. The UHV chamber was equipped with a water-cooled Knudsen boron nitride effusion cell for Si homo epitaxy. The deposition rate was 1 ML/min (1 ML = 7.8×10^{14} cm^{-2}, the site density of the unreconstructed Si(111) plane). The STM is a commercial large sample type from Omicron. Electrochemically etched (2 M NaOH) single crystalline W⟨100⟩ and hand cut PtIr tips have been used which were out gassed and flash annealed in UHV. The images were recorded at room temperature in the constant current mode at voltages ranging between −3.0 V and +3.0 V and a current between 0.01 nA and 0.05 nA. All given voltages are referring to the substrate polarity, the tip was grounded. Scanning tunneling spectroscopy (STS) spectra were obtained by measuring the tunnel current I vs the voltage V across the tunnel junction.

The resistivity experiments were performed at a base pressure of 1×10^{-8} Pa in a LAS-630 spectrometer equipped with AES, LEED and a home made variable temperature (40–1200 K) sample holder. A four contact geom-