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Effective mass of a two-dimensional $\sqrt{3} \times \sqrt{3}$ Ga single atomic layer on Si(111)

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ABSTRACT

The effective mass of the empty conduction band surface state of a single atomic $\sqrt{3} \times \sqrt{3}$ Ga layer on Si(111) is determined using scanning tunneling spectra. The methodology is based on calculating the tunnel current using its dependence on the effective density of state mass and a parabolic band approximation followed by fitting to the measured tunneling spectra. An effective mass of $m_{\text{eff,C}} = 0.59 \pm 0.06$ is obtained, in good agreement with a band structure calculation and inverse photo electron spectroscopy data.

1. Introduction

Future semiconductor devices are likely to rely heavily on nanostructures. Therefore the transport of charge carriers in semiconductor nanostructures is attracting increasing interest. In a semi classical approach, the transport of charge carriers is primarily governed by the effective mass tensor of electrons and holes. Neglecting the crystal anisotropies, the scalar effective mass m^* is reasonably well known for most bulk materials. The effective masses m^* range typically from almost zero [1] to several hundred times the rest electron mass (m_e) [2] in the bulk. However, with ongoing miniaturization of semiconductor devices and the trend towards the use of nanostructures, the increasing surface to volume ratio reduces the relative fraction of bulk material. Hence, transport in semiconductor nanostructures is to a large degree determined by surface and/or interface effects, where little is known about the effective masses.

The knowledge of the dispersion relation $E(k)$ is crucial for the determination of the effective mass. Angle-resolved photoemission spectroscopy (ARPES) delivers information of the momentum and energy, but it is hardly applicable on individual nanostructures. Although scanning tunneling spectroscopy (STS) is ideally suited for probing the local density of states of an individual nanostructure by evaluating the derivative dI/dV of the tunnel current with respect to the tunnel voltage V, it is a very difficult task to quantitatively measure the involved k vectors and hence the dispersion relation. Only in special cases information about the k vectors of the tunneling electrons can be derived from scanning tunneling microscope (STM) measurements: First, one can extract the parallel wave vector $k_\parallel$ of the tunneling electrons from the decay of the local density of states into the vacuum [3–6], since the decay constant κ depends on $k_\parallel$ [7,8]. This method is, however, not yet precise enough to provide quantitative dispersion relations. Second, the wavelength of standing waves present on metallic surfaces is used to derive quantitatively the dispersion relation [9,10]. However, most of the semiconductor surfaces do not exhibit standing electron waves and thus this method is restricted to some special cases.

Therefore, we illustrate here a methodology applicable to individual semiconducting nanostructures for extracting effective masses of a two dimensional $\sqrt{3} \times \sqrt{3}$ Ga single atomic layer on Si(111) from scanning tunneling spectra. The dependence of the tunnel current on the effective density of states mass is utilized to extract the effective mass of empty and filled surface states by fitting calculated to measured tunneling spectra.

2. The effective mass in STS

In order to obtain the effective mass from STS, we recall the relation of the effective mass and the tunnel current: For density of states (DOS) calculations of a d-dimensional system, the effective density of states mass $m_{\text{eff,DOS}}$ is derived from the scalar effective mass of the band $m^* = m_{\text{eff}} \cdot m_e$ using

$$m_{\text{eff,DOS}} = g^{\frac{2}{d}} \cdot m_{\text{eff}}. \quad (1)$$

The degeneracy factor g is the number of equivalent band extrema [11]. The tunnel current can be calculated following the model of Bono and Good [12] applied to semiconductors [8], using a parabolic approximation of the dispersion relation with the effective density of states

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mass $m_{\mathrm{eff,DOS}}$. The parabolic approximation is suitable for wave vectors near the valence-band maximum or the conduction-band minimum. The tunnel current between tip and semiconductor is then given by [8, 12]:

$$I = \pi R^2 \frac{4\pi e m_e}{h^3} \left(\int_{E_F}^{E_F - eV} dE\ \theta\ (E - EC)^* \int_{E}^{e\overline{\Phi}} dW T(W) \right) \tag{2}$$

with the transmission probability $T(W)$

$$T(W) = exp\left(-\sqrt{\frac{8m_e}{\hbar^2}} \int_{z_1}^{z_2} \sqrt{B(z) - W} dz \right). \tag{3}$$

The tunneling area is approximated by Bono and Good with πR^2, where R is the radius of the tip [12]. We use for this 1 nm^2 following Feenstra and Stroscio [8]. E_F and E_C correspond to the Fermi energy and the conduction band edge of the semiconductor, respectively. z_1 (z_2) corresponds to the position of the sample surface (tip). $B(z)$ is the barrier potential in the vacuum gap between the tip and the surface as defined by Ref. [8,12]. $e\overline{\Phi}$ is given by

$$e\overline{\Phi} = \left(1 - m_{\mathrm{eff,DOS}}\right) E + m_{\mathrm{eff,DOS}} \cdot E_C. \tag{4}$$

Note that we assume that the tunneling probability is not changed by non-zero parallel wave vectors of the tunneling electrons. At room temperature the momentum transfer can be accommodated by surface phonons. The dispersion of the surface phonon shows branches at low energy (<10 meV) covering all k vectors [13,14]. Hence, the energy loss of the tunneling electrons is negligible compared to the thermal energy resolution at room temperature of ~100 meV. This assumption is supported by the observation of normal tunnel current even for electrons tunneling into or out of states at the edge of the surface Brillouin zone [6].

3. The investigated system

The $\sqrt{3} \times \sqrt{3}$ Ga overlayer on a Si(111) was prepared by evaporating approximately 0.33 monolayers of Ga on a previously cleaned and degassed 7 × 7 reconstructed Si(111) surface at ~750 K, followed by a slow cool down to room temperature [15]. The STM measurements were performed at room temperature using electrochemically etched tungsten tips.

The geometrical structure of the $\sqrt{3} \times \sqrt{3}$ Ga overlayer on Si(111), illustrated in Fig. 1a and b, is analogous to that of the $\sqrt{3} \times \sqrt{3}$ Al on Si(111) calculated by Northrup [16]: The Ga adatoms are located at so-called T_4 sites centered above three Si atoms in the uppermost substrate layer. The bond length between the adatoms and the substrate Si atoms is 2.5 Å [16]. The Ga adatoms cause a downward displacement of the first and second layer Si atoms by 0.0265 Å and 0.334 Å, respectively [16]. Taking into account these displacements, one can derive the distance perpendicular to the surface between the Ga adatoms and the first layer of Si substrate atoms to be $\Delta_{12} = 1.363$ Å(Fig. 1b).

4. Experimental results

Fig. 1(c) shows a filled state STM image of the $\sqrt{3} \times \sqrt{3}$ Ga overlayer on the Si(111) substrate. Each maximum corresponds to one Ga or Si adatom [15]. The brighter maxima arise from Si adatoms at $\sqrt{3} \times \sqrt{3}$ adatom sites [17], acting as dopants [15]. At negative voltage their localized state in the band gap contributes to a locally higher tunnel current, which leads to the difference in brightness compared to the Ga atoms: Fig. 2 shows atomically resolved tunneling spectra measured above Ga (filled blue squares) and Si atoms (red filled circles). The Si adatoms exhibit a pronounced localized state in the gap at negative voltages. The resulting tunnel current is one to two orders of magnitudes larger above Si adatoms than above Ga adatoms.

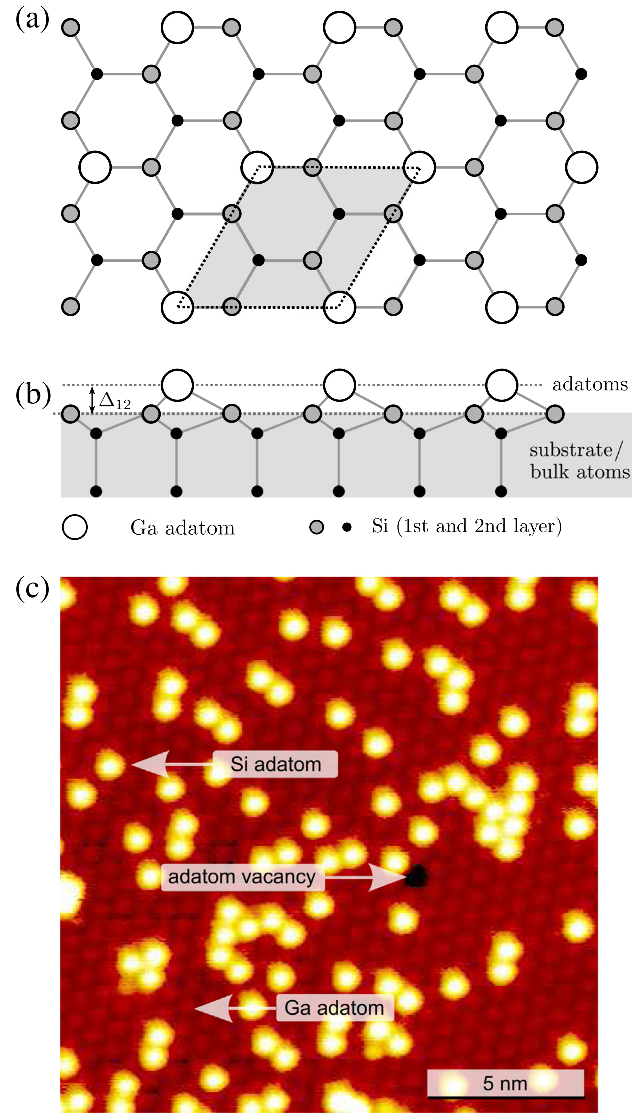

Fig. 1. (a) Schematic top view of the $\sqrt{3} \times \sqrt{3}$ Ga–Si(111) structure. The unit cell of the Ga overlayer is indicated by the gray shaded area. (b) Side view. The gray shaded area marks the substrate. The distance perpendicular to the surface between the Ga adatoms and the first layer of Si substrate atoms is given by Δ_{12}. (c) Constant-current STM image of the filled states of the $\sqrt{3} \times \sqrt{3}$ Ga–Si(111) structure measured at −2.0 V. Bright spots represent Si adatoms on $\sqrt{3} \times \sqrt{3}$ Ga sites.

Since the tip is not perfectly point-shaped, the $I(V)$ spectra obtained above Ga adatoms are also slightly influenced by the localized Si states in the band gap region. This shows up as a slight increase of the tunnel current at negative voltages, near the valence band edge, as can be seen in Fig. 2. Subtracting this background (solid gray line) the pure valence band current is obtained (I_V). The resulting band gap agrees well with that of Si. Due to the presence of the filled gap state at Si adatoms, we concentrate here on the empty conduction band states at Ga sites only, where the influence of the Si adatoms can be neglected. In order to minimize the influence of the Si adatoms on the tunnel current further, no tunneling spectra from Ga sites with nearest neighbor Si adatoms were used. This allows to reduce the influence of the Si adatoms by about 2 orders of magnitude, since the gap state of the Si adatoms is spatially highly localized [6]. Such tunneling spectra, acquired above many Ga adatom sites, were selected and averaged.