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Unpinning of the Fermi level at clean (111)A surfaces of heavily Si-doped $In_{0.53}Ga_{0.47}As$ thin films epitaxially grown on InP substrates

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1. Introduction

The existence of Fermi level pinning remains a major obstacle for the realization of a high-performance metal-insulator-semiconductor field-effect transistor (MISFET) based on $In_xGa_{1-x}As$ ($0 \le x \le 1$), in spite of considerable effort to develop passivating coatings [1]. It is well known that the Fermi level of (001) oriented $In_{0.53}Ga_{0.47}As$ crystals is pinned in the band gap both at interfaces with metal or insulators [2] and at clean surfaces [3,4]. Here, we show that the Fermi level is unpinned at clean (111)A surfaces of heavily Si-doped $In_{0.53}Ga_{0.47}As$ thin films epitaxially grown on InP substrates.

2. Experiment

100-nm-thick $In_{0.53}Ga_{0.47}As$ thin films doped by Si were grown by molecular beam epitaxy (MBE) on lattice-matched semi-insulating InP(111)A substrates. Samples were then transferred under ultra-high vacuum (UHV) to a low-temperature scanning tunneling microscope (LT-STM), operating at liquid helium temperature. Since semi-insulating substrates were employed, grown thin films were made in direct electrical contact with the STM stage in order to apply a bias voltage V between the tip and the sample surface. STM topographs and differential conductance (dI/dV) maps were realized in the constant-current mode. Scanning tunneling spectroscopy (STS), i.e. current I and dI/dV as a function of sample voltage V, was obtained in the constant-height mode. dI/dV is known to be proportional to the local density of states (LDOS) at the surface, at energy $E_F + eV$ (where E_F is the Fermi level). After STM investigations, the free-electron concentration n_e (sheet free-electron density divided by the grown $In_{0.53}Ga_{0.47}As$ thickness) and the Hall mobility of the same $In_{0.53}Ga_{0.47}As$ thin films were determined by the Van der Pauw method at room temperature. The values of n_e measured by the Van der Pauw method show a consistent variation with Si concentrations measured by secondary ion mass spectrometry (SIMS). Hall mobilities were 5000 $cm^2.V^{-1}.s^{-1}$ and 2900 $cm^2.V^{-1}.s^{-1}$, for $n_e = 8.0\times10^{16}$ cm^{-3} and $n_e = 1.3\times10^{19}$ cm^{-3}, respectively. These mobilities are comparable to that reported for Si-doped $In_{0.53}Ga_{0.47}As$ thin films grown by MBE at optimized conditions on InP(001) substrates [5]. It means that the crystal quality of the grown thin films used in our experiments was very high.

3. Results and discussion

Fig. 1 shows LDOS spectra by STS at the (111)A clean surface of n-type high-quality $In_{0.53}Ga_{0.47}As$ thin films, for different values of n_e. The dI/dV spectra yield to a band gap of about 800 meV, in agreement with the value measured on $In_{0.53}Ga_{0.47}As$ at 7 K by photoluminescence [6]. The dI/dV spectra also indicate that the surface Fermi level increases with increasing n_e, from $E_F - E_{Csurf} = +\ 70$ meV for $n_e = 8.0\times10^{16}$ cm^{-3}, to $E_F - E_{Csurf} = +\ 200$ meV for $n_e = 1.3\times10^{19}$ cm^{-3} (E_{Csurf} is the bottom of the conduction band at the surface). Fig. 2 shows a plot of the surface Fermi level position, determined by STS, as a function of n_e. The surface Fermi level is pinned in the conduction band ($E_F - E_{Csurf} = +\ 70$ meV) at low values of n_e. However, at values of n_e higher than 10^{18} cm^{-3}, the surface Fermi level increases with increasing n_e, indicating an unpinning phenomenon. It is completely different from the case of the (001) crystal orientation, where the surface Fermi level is always pinned in the band gap [3,4].

By calculating the bulk Fermi level positions, it was found that the band bending at the (111)A surface is upward (downward) for n_e higher (lower) than 7×10^{17} cm^{-3}. Calculations based on a triangular potential approximation show that there is no two-dimensional state formed in the case of downward band bending.

In order to confirm the n_e-dependence of the Fermi level position at the (111)A surface, electron standing waves were imaged by dI/dV mapping. Fig. 3 shows dI/dV maps at a sample voltage $V = +\ 250$ mV, for different values of n_e ($n_e > 1.7\times10^{18}$ cm^{-3}). For these doping concentrations, the band bending at the surface is upward, and the grown $In_{0.53}Ga_{0.47}As$ thickness (100 nm) is larger than the bulk Fermi wavelength (17 nm for $n_e = 1.7\times10^{18}$ cm^{-3}). Therefore, conduction-band electrons can be considered as a three-dimensional electron gas (3DEG). The LDOS spatial modulation observed in dI/dV maps is ascribed to 3DEG standing waves, mainly due to scattering at dopants [7]. As also shown in Fig. 3, fast Fourier transform (FFT) power spectra of dI/dV maps can be employed to extract the 3DEG wave number k [7]. In the case of 3DEG standing waves, a FFT power spectrum of a LDOS map corresponds to the projection of a constant-energy surface on the plane $k_z = 0$ (where k_z is the wave number in the direction perpendicular to the surface). Therefore, the diameter of the circular contour of the disc-shaped distribution in a FFT power spectrum corresponds to $4k$. According to the FFT power spectra of Fig. 3, k at a fixed sample voltage increases with increasing n_e, which means that the surface Fermi level increases with increasing n_e.

For a more quantitative analysis, the dispersion relation of the conduction band was established experimentally at different values of n_e, by extracting the 3DEG wave number k from dI/dV maps as a function of sample voltage V. The dispersion relation is well described by a **k.p** theory model, including non-parabolicity of the conduction band. At each value of n_e which was investigated, the fit led to an electron effective mass at the bottom of the conduction band consistent with a previously reported value of 0.041 m_0 [8], and to a surface Fermi level position comparable to the value extracted from STS.

4. Conclusion

The Fermi level position at the n-type $In_{0.53}Ga_{0.47}As(111)A$ clean surface was consistently determined both by STS and dI/dV mapping of electron standing waves. At Si-doping concentrations higher than 10^{18} cm^{-3}, the surface Fermi level was found to increase with increasing free-electron concentration, indicating an unpinning phenomenon.

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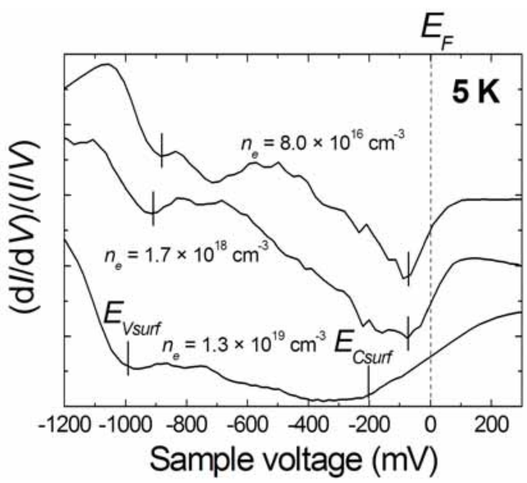

FIG. 1. LDOS spectra obtained by constant-height STS at the $In_{0.53}Ga_{0.47}As(111)A$ surface, for different free-electron concentrations n_e (5 K). E_F is the Fermi level. E_{Vsurf} and E_{Csurf} are the top of the valence band and the bottom of the conduction band at the surface, respectively.

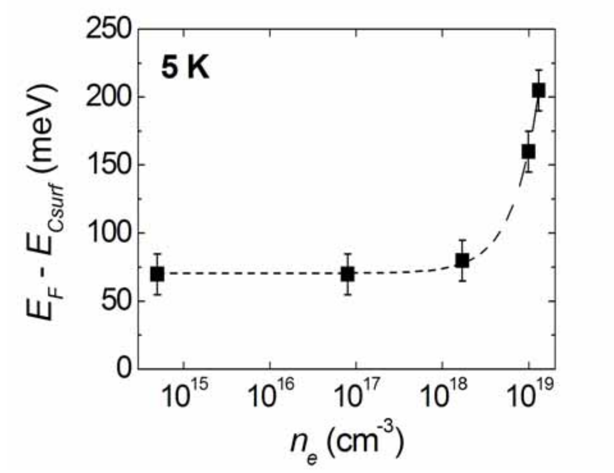

FIG. 2. Fermi level at the $In_{0.53}Ga_{0.47}As(111)A$ surface, determined by STS, as a function of free electron concentration n_e (5 K). The dashed line is a guide for the eye.

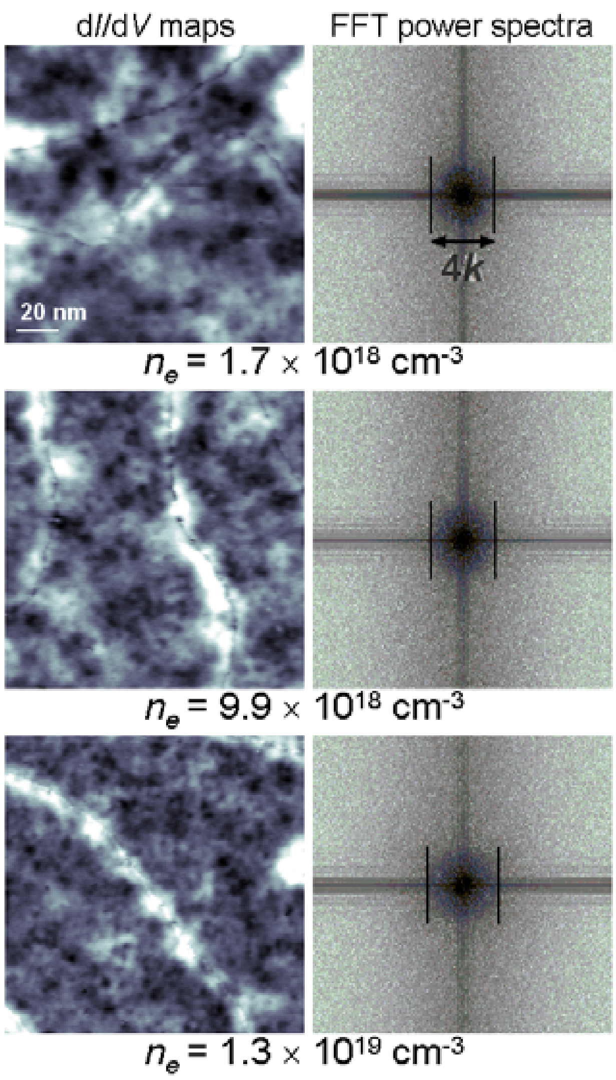

FIG. 3. 134 nm × 134 nm constant-current dI/dV maps at the $In_{0.53}Ga_{0.47}As(111)A$ surface, at a sample voltage V = + 250 mV, for different free-electron concentrations n_e (5 K). FFT power spectra of the dI/dV maps are also shown. The diameter of the circular contour of the disc-shaped distribution in a FFT power spectrum corresponds to 4k, where k is the 3DEG wave number.