Direct measurement of quantum-state dispersion in an accumulation layer at a semiconductor surface

V. Yu. Aristov* and G. Le Lay
CRMC2-CNRS, Campus de Luminy, Case 913, 13288 Marseille Cedex 09, France and UFR Sciences de la Matière, Université de Provence, Marseille, France

V. M. Zhilin
Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow district 142432, Russia

G. Indlekofer, C. Grupp, and A. Taleb-Ibrahimi
LURE, Université de Paris-Sud, Bâtiment 209 D, 91405 Orsay Cedex, France

P. Soukiassian
Commissariat à l'Energie Atomique, DSM-DRECAM-SRSIM, Bâtiment 462, Centre d'Etudes de Saclay, 91191 Gif sur Yvette Cedex, France and Département de Physique, Université de Paris-Sud, 91405 Orsay Cedex, France

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We use high-resolution photoemission spectroscopy to measure the dispersions of quantized energy levels located in an accumulation two-dimensional electron channel created in the subsurface region of a semiconductor. The experiments are performed for InAs(110) covered by about 10^{-2} Cs monolayer. From the band dispersion, the average effective mass of the carriers in the channel is determined. Our findings are further supported by self-consistent calculations and model-function curve fitting. [S0163-1829(99)07735-8]

The characterization of electron accumulation and inversion layers at interfaces formed with narrow band-gap III-IV semiconductors, particularly InAs, was pioneered by Tsui.[1] Recent studies, now performed directly at the surface of such III-IV semiconductors, have generated considerable renewed interest.[2–7] Indeed InAs and InSb belong to this class of semiconductors which present rather unique properties, such as high carrier densities, even at very low temperatures, and extremely high electron mobilities. These exceptional properties are potentially very promising for a new family of devices able to operate in conditions where the carriers of other semiconductors are frozen. A typical application could be, for example, the planet Mars exploration. As for other III-V semiconductors, well cleaved InAs(110) samples present no surface states in the fundamental gap, thus exhibiting flat band conditions up to the very surface. However, we discovered recently that a small amount of alkali metals ($\sim$0.01 monolayer) adsorbed on the InAs(110) surface at room temperature (RT) leads to a strong downward band bending which can result in a pinning of the Fermi level (E_F) at the surface as high as up to 0.6 eV above the conduction-band minimum (CBM) for both types of bulk doping, thus creating inversion or accumulation layers just beneath the top surface.[8,9] If the mobility of the carriers is sufficient, these layers could behave as two-dimensional (2D) electron channels in the vicinity of the surface. Because these channels are situated just below the free surface, they can be studied by direct photoemission. We showed in a previous study, performed at room temperature (RT), that a small photoemission feature appearing near E_F in the close vicinity of the $\overline{\Gamma}$ points of the first and second Brillouin zones after adsorption of $\sim$0.01 monolayer (ML) of cesium, corresponded to emission from such a two-dimensional (2D) electron channel.[9] We further proved that this feature arose from the emission from two occupied discrete energy levels within the channel, resulting from quantization along the surface normal. Due to the very narrow phase space where this emission could be detected and the comparatively large angular aperture of the photoelectron analyzer this photoemission feature was, as a matter of fact, essentially measured in an angle-integrated mode. The angle-integrated density of states of a 2D system is constant; consequently, in the situation of several occupied energy levels, the corresponding photoemission spectrum should present a staircaselike shape.

One of the essential parameters for low-temperature devices is the carrier mobility which requires the knowledge of the effective mass. The latter is still unknown for this very promising system.

In this Brief Report, we present the first dispersion of these quantized electronic states in k space for Cs/InAs(110) and determine the average electron effective mass in the 2D channel. The experiment was successfully achieved via a drastic reduction of the analyzer aperture (to increase the angular-momentum resolution) and by decreasing the temperature at 30 K (to reduce phonon broadening). The experimental results are in excellent agreement with self-consistent calculations.

The synchrotron radiation photoemission experiments are performed at the Laboratoire d'Utilisation du Rayonnement Electromagnetique (LURE, Université de Paris-Sud/Orsay) using the soft-x-ray light emitted by the Super ACO storage ring and dispersed by a high-resolution toroidal grating monochromator at the SU3 beam line. The photoelectron energy is analyzed by an angle-resolved hemispherical electrostatic analyzer with an acceptance angle reduced close to ±0.5°. Low-temperature (~30 K) measurements allowed an overall energetic resolution of ~35 meV. The pressure in the experimental system during data acquisition is always better than 7×10^{-11} Torr. Clean InAs(110) surfaces are obtained by cleaving *in situ* *n*-type (S doped, $\sim3\times10^{17}\,\mathrm{cm}^{-3}$) InAs single-crystal bars. Pure Cs is condensed onto the InAs(110) surfaces at room temperature from a properly outgassed SAES Getters source, without detectable pressure increase during deposition. Band bending was measured from the In $4d$ core-level shifts; we checked that they were the same at room temperature and 30 K, which ensures that the doping level was sufficient to avoid any spurious surface voltage effect. The E_F position is taken from the Cu sample holder. The photoemission measurements are performed at a photon energy of $h\nu=8$ eV, sufficiently low to yield enough signal from the subsurface 2D electron channel, due to the very low kinetic energies and, as a consequence, high escape depths of the outgoing photoelectrons.[9]

Let us first discuss the shapes of the photoelectron spectra expected for the 2D channel at different analyzer acceptance angles, i.e., for different momentum resolutions. Figure 1(a) (right side) displays schematically a potential well resulting from a downward band bending for an *n*-type sample and the positions of the first two energy levels relative to E_F within the 2D electron channel. The left side of the figure shows the dispersions of these levels in *k* space along the component of the momentum parallel to the surface. The right side of Fig. 1(b) shows the integrated density of the two filled states (hatched staircase). The staircaselike overall shape would be that of a spectrum recorded at 0 K with an analyzer acceptance angle $\Delta\Theta_a$, corresponding in *k* space to $\Delta k_a \geqslant k_0$ (k_0 is the momentum at the Fermi energy for the ground state). In the opposite case of a very narrow acceptance angle $\Delta\Theta_a$, corresponding in *k* space to $\Delta k_a \ll k_1$ (k_1: momentum at the Fermi energy for the level E_1) one should obtain the discrete spectrum shown in Fig. 1(c), i.e., one should detect two narrow isolated peaks instead of the continuous staircaselike construction. An intermediate case where the analyzer acceptance is close to the angular width of the emission from the 2D channel is shown in Fig. 1(d). Of course a real experimental spectrum is influenced by the nonzero temperature and the limited energy resolution of the spectrometer.

We perform self-consistent calculations giving the potential well shape, the electron-energy levels, and the charge distribution below the surface (following an approach similar to that of Ref. 10). We use parameters corresponding to our actual experimental conditions: doping $n\sim3\times10^{17}\,\mathrm{cm}^{-3}$, E_F position at 0.4 eV above the CBM and $T=30$ K. Three occupied energy levels are found at $k=0$ in the well, respectively, at $E_0=167$ meV, $E_1=64$ meV, and $E_2=23$ meV below E_F. The total charge density is zero at the very top surface (as expected for a quantized electron gas) and reaches a maximum of $N_s=2.14\times10^{18}$ electrons/cm^3 at a distance of approximately 52 Å below the very surface.

We now investigate the quantized states dispersion using photoemission in the vicinity of the center of the first Brillouin zone (normal emission) at 30 K (Fig. 2). We clearly observe emission coming from two peaks located just below E_F, in a narrow angular range of $\sim\pm2.5°$ from the surface normal. It is interesting to notice the close resemblance of these experimental spectra with those depicted in Figs. 1(c) and 1(d). Moreover, the dispersion of these peaks can be followed by a simple visual inspection. However, because of the proximity of the second peak to the Fermi level that might cause some error in the determination of its maximum,

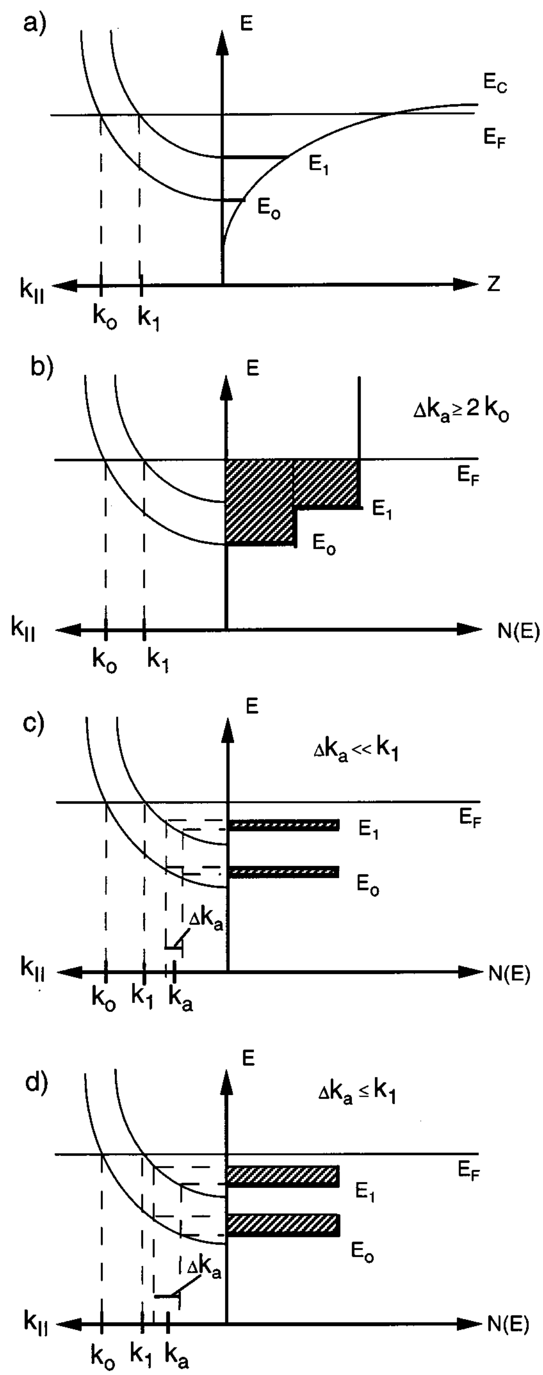

FIG. 1. Schematics of (a) a downward band bending for an *n*-type sample (right side) and the positions (relative to E_F) of the first two energy levels of the resulting 2D electron channel; the left side shows the expected dispersions of these two levels in *k* space; (b) the integrated density of filled states (right side), illustrated by the hatched staircase, expected at $T=0$ K, for a "large" acceptance angle of the analyzer; (c) the angle-resolved density of filled states (right side) expected for a very small acceptance angle of the analyzer; (d) an intermediate situation.

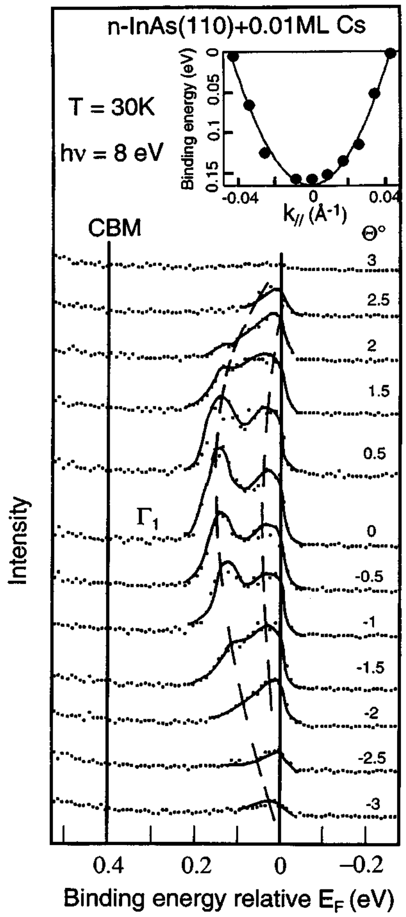

FIG. 2. Photoemision spectra taken from the 2D electron channel at different emission angles along the $\bar{\Gamma}$-$\bar{X}$ direction (⟨100⟩ direction in real space) in the vicinity of the $\bar{\Gamma}$ point of the InAs (110) surface. The solid lines are drawn to guide the eyes through the experimental points. The inset shows the electronic state energy dispersion as a function of $k_{\parallel}$ (black dots).

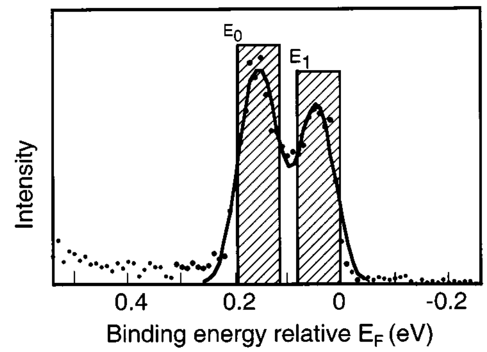

FIG. 3. Best model-function fitting curve (solid line) to the normal-emission spectrum of Fig 2 (dots); rectangles show the ''ideal'' effective densities of states for a two subband model of the degenerated 2D quantized accumulation channel.

we restrict the evaluation of our data set to the dispersion of the ground-state level (E_0) (peak position in binding energy versus parallel wave vector for each emission angle), which is shown as an inset in Fig. 2. The data points can be well fitted by a parabola in this narrow k range at the bottom of the conduction band, although, indeed, InAs has an overall strongly nonparabolic conduction band.[11] From this curve, we derive the effective mass of the electrons in the 2D channel for motion parallel to the surface: $m^* = 0.05 m_0$ (m_0 is the free-electron mass), while the bulk value at the CBM is $0.023 m_0$.[11]

Taking into account two filled levels (we were able to resolve only two filled levels because level E_2 is too close to E_F to be detected), we can synthesize the overall photoemission spectrum at normal emission for such a 2D system. Since we do not know the real aperture function of our analyzer, we assume, for simplicity, that it has a rectangular shape, i.e., all photoelectrons escaping from the surface within an angle $\Delta\Theta_e$ inferior to $\Delta\Theta_a$ are effectively counted, while all other photoelectrons emitted outside of this small-angle region are not detected. At normal emission, the photoelectron path deviation from the analyzer optical lens axis is a function of the kinetic energy; hence, within $\Delta\Theta_a$, an angle-averaged 2D density of states is measured. Since it is constant, each of the measured filled levels in the photoemission energy distribution curve (EDC) should be represented by a rectangle. The higher binding-energy side of each filled rectangle state should correspond to $k_{\parallel} = 0$, while its lower binding energy side should be set either at the energy corresponding to the maximum deviation $\Delta\Theta_a/2$, i.e., $\Delta k_a/2$, or at the Fermi level energy E_F, if $\Delta k_a/2 \geqslant \mathbf{k}_0$ (see Fig. 1). The density of states being the same for both levels, the heights of these rectangles should be equal. However, as shown in Ref. 9, the electron densities of each level are localized at different distances below the surface resulting in somewhat different attenuations of the photoelectron currents inside the sample, before escaping from the very surface, and thus in different measurable intensities, as shown in Fig. 3. The consideration of the cutoff by the Fermi function at 30 K, the temperature of our measurements, and the spreading due to the instrumental function (assumed to be a Gaussian contribution), results in the solid curve of Fig. 3, which has been adjusted to give the best fit to the experimental spectrum. From the fit, the following optimized free parameters are derived for the positions of the energy levels and the instrumental function: $E_0 = 184$ meV, $E_1 = 100$ meV, Gaussian full width at half maximum is 52 meV. Note that the instrumental function deduced from this fitting procedure is larger than our total resolution (35 meV), obtained from Fermi-step measurements; this is correct since, here, we must additionally take into account the energy spread resulting from the (unknown) angle aperture function. Despite all the assumed simplifications, we nevertheless obtain a rather fair agreement with the previously calculated values of the energy levels (see above). The larger difference between the theoretically calculated energy position of the energy level E_1 and that derived from the fitting procedure, as compared to the case of E_0, is not surprising since the contribution of the other filled level E_2, very close to E_F, has been neglected and also since the escape cone effects mentioned above are only roughly taken into account in this synthesis.

To summarize, we have performed a direct measurement of a quantized two-dimensional electron accumulation channel created below the InAs(110) surface by adsorption of a small amount of cesium using photoemission spectroscopy at low temperatures. We have individually resolved the discrete energy levels within the channel and measured their dispersion as a function of the component of the momentum parallel to the surface. From the dispersion we have determined the carrier effective mass within the channel. Self-consistent calculations and model-function adjustment to the experimental normal-emission spectrum yield positions of the energy levels in agreement with the experimental ones.

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*On leave from Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow district, 142432, Russia.

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