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P. Krispin, A. Knauer, and S. Gramlich

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Polarization charges at spontaneously ordered (In, Ga)P/GaAs interfaces

P. Krispin[a)]
Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

A. Knauer and S. Gramlich
Ferdinand-Braun-Institut für Höchstfrequenztechnik, Albert-Einstein-Strasse 11, 12489 Berlin, Germany

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The depth-resolved electrical characteristics of *n*- and *p*-type GaAs/(In, Ga)P/GaAs heterojunctions are examined by capacitance–voltage measurements. Different epitaxial growth conditions are chosen to produce heterointerfaces with (In, Ga)P layers of various degrees of order. Irrespective of the conduction type of the heterojunction studied, we find positive [negative] sheet charges at the (In, Ga)P-on-GaAs [GaAs-on-(In, Ga)P] interfaces. The density of both interfacial charges increases with increasing degree of (In, Ga)P order. The experimental results can be completely explained by taking into account the spontaneous polarization of ordered (In, Ga)P. The polarization difference between ordered (In, Ga)P and GaAs (no polarization) results in opposite sheet charges at the two complementary interfaces with GaAs, in accordance with theoretical predictions. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1467978]

For electronic devices, the lattice-matched (In, Ga)P/GaAs heterointerface is a real alternative to the (Al, Ga)As/GaAs system, because it is not affected by the affinity of Al to oxygen and donor-related traps (*DX* centers). Despite many investigations, the features of (In, Ga)P/GaAs interfaces are still controversially discussed. Since spontaneously ordered (In, Ga)P exhibits a strong polarization,[1–3] the electronic characteristics of (In, Ga)P/GaAs heterojunctions may be largely modified. Sheet charges and related electric fields are, for example, expected at interfaces between GaAs (no polarization) and ordered (In, Ga)P. So far, however, the influence of (In, Ga)P ordering on the interfacial properties has attracted only little attention.[4–6]

The presence of sheet charges at the (In, Ga)P/GaAs interface may, e.g., substantially alter the offset values as determined by several experimental techniques. Methods like photoluminescence (PL) spectroscopy of GaAs quantum wells in (In, Ga)P,[7,8] ballistic-electron emission microscopy,[4] photoemission, and current–voltage characteristics of heterojunctions,[9–15] which have been applied to measure the band offsets at (In, Ga)P/GaAs interfaces, rely crucially on the assumption that the band diagram is not influenced by sheet charges. The related offset values are, therefore, not always reliable.

In contrast, capacitance versus voltage ($C-V$) studies with metal–semiconductor (MS) contacts on isotype heterojunctions are known to independently provide values for the band offset as well as for the sheet charge density.[16,17] In this letter, we therefore use $C-V$ measurements to examine the electrical properties of (In, Ga)P/GaAs interfaces grown by metalorganic vapor-phase epitaxy (MOVPE). Samples with (In, Ga)P layers of various degrees of order are produced by different growth conditions.[6] It is shown that the polarization of spontaneously ordered (In, Ga)P gives rise to positive and negative sheet charges at the (In, Ga)P-on-GaAs (normal) and the GaAs-on-(In, Ga)P (inverted) interfaces, respectively.

For the (In, Ga)P-on-GaAs interface of *n*-type heterojunctions with different degrees of order, typical depth profiles of the electron concentration *n* are depicted in Fig. 1. Since long-range ordering leads to a band-gap reduction of (In, Ga)P,[18,19] the PL peak energy shifts accordingly (see, the inset of Fig. 1). Neglecting the exciton binding energy and Stokes shift, the PL peak energy measured at 10 K can be used as a measure for the band gap of the differently ordered (In, Ga)P layers. The degree of order η is calculated from the relation $E_G(0)-E_G(\eta)=0.471\ \eta^2$ (eV), which has been experimentally verified.[18] $E_G(\eta)$ denotes the band gap of

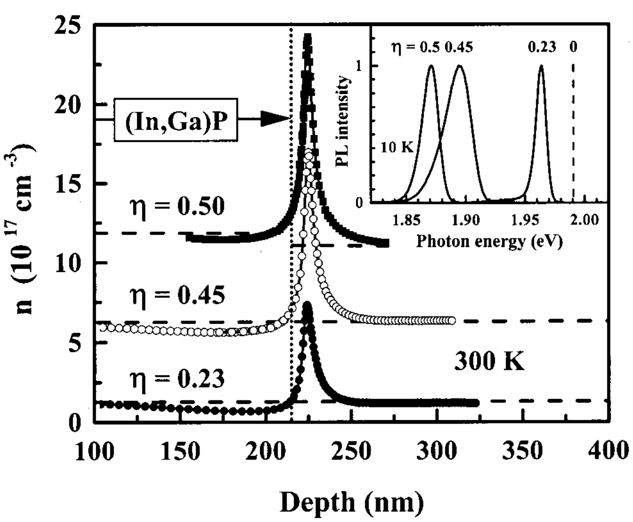

FIG. 1. Typical depth profiles of the electron concentration *n* for (In, Ga)P-on-GaAs interfaces measured at 300 K and 1 MHz. Different order parameters η correspond to different MOVPE growth conditions. The depth scales are normalized to an interface position of 215 nm (marked by the vertical dotted line). Horizontal dashed lines denote the doping levels in GaAs and (In, Ga)P. Curves are vertically shifted for clarity. In the inset, the PL spectra of the (In, Ga)P layers are plotted. For $\eta=0$, the PL peak position is indicated by a vertical dashed line.

[a)]Electronic mail: krispin@pdi-berlin.de

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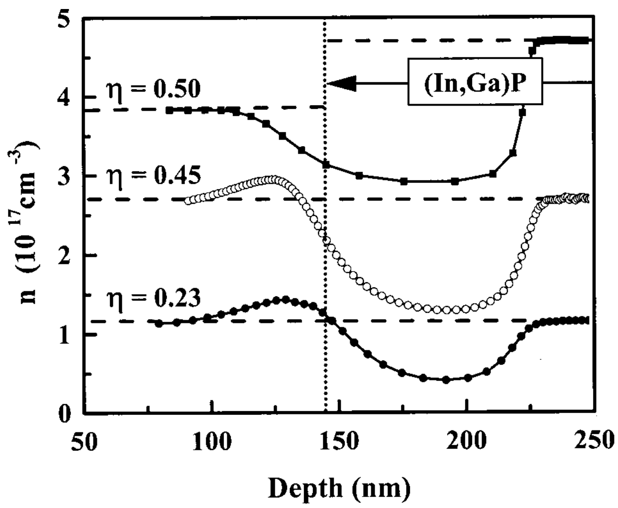

FIG. 2. Typical depth profiles of the electron concentration n for the GaAs-on-(In, Ga)P interfaces of the same heterostructures as in Fig. 1 measured at 300 K and 1 MHz. The depth scales are normalized to an interface position of 145 nm (marked by the vertical dotted line). Horizontal dashed lines denote the doping levels in GaAs and (In, Ga)P. Curves are vertically shifted for clarity. Note the other depth scale and different offsets compared with Fig. 1.

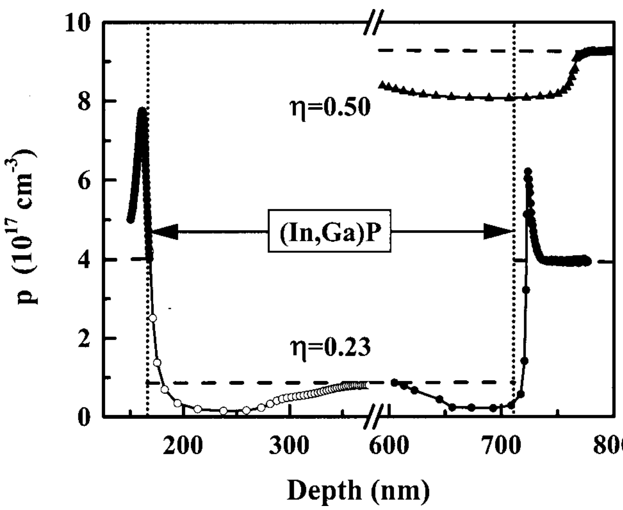

FIG. 3. Depth profiles of the hole concentration p for GaAs/(In, Ga)P/GaAs heterojunctions measured at 300 K and 1 MHz. The two different order parameters η correspond to different MOVPE growth conditions. The curves are vertically shifted for clarity. The interface positions are marked by vertical dotted lines. Horizontal dashed lines denote doping levels in GaAs and (In, Ga)P. For the $\eta = 0.23$ sample, multiple recess-etch steps are distinguished by different symbols.

(In, Ga)P with order parameter η. The degree of order varies from $\eta = 0$ for complete disorder to $\eta = 1$ for perfect ordering. $E_G(0)$ is found to be 1.99 eV.

The common valley/peak structure of isotype heterojunctions is revealed for all order parameters studied. Electron depletion and accumulation are observed on the (In, Ga)P and GaAs sides, respectively. It is evident that the conduction-band edge in (In, Ga)P is higher than in GaAs. Whereas the depletion region on the (In, Ga)P side of the heterointerface remains practically unchanged, the peak concentration on the GaAs side becomes higher with increasing η. When integrating each curve in Fig. 1, an excess of electrons over the doping level is found, which reaches 1.2×10^{12} cm^{-2} for the interface with highly ordered (In, Ga)P. This surplus of electrons is due to positive sheet charges, which lower the conduction-band edge at the normal interface. The density of positive charges at the (In, Ga)P-on-GaAs interface is apparently related to the order parameter η of the (In, Ga)P layer.

For the GaAs-on-(In, Ga)P interface of the n-type heterostructures, that have been studied in Fig. 1, the depth profiles of the electron density are plotted in Fig. 2. The typical valley/peak structure of isotype heterojunctions is again present. In contrast to the normal interfaces, the peak concentration on the GaAs side of the inverted interfaces is lower and decreases for higher-ordered (In, Ga)P. When the depletion becomes dominant for $\eta = 0.50$, the electron accumulation on the GaAs side is missing. For n-type inverted interfaces, we always find a distinct electron depletion. For the samples in Fig. 2 with η values of 0.23, 0.45, and 0.50, the electron deficits are found to be about 3×10^{11}, 9×10^{11}, and 13×10^{11} cm^{-2}, respectively. The electron depletion is due to negative charges, which lead to an elevated conduction-band edge at the interface. The density of these charges at the inverted interface corresponds apparently to the degree of (In, Ga)P order. Interfacial electron traps were not observed and can, therefore, be neglected as a possible source of negative sheet charges.[6]

For two p-type heterojunctions with differently ordered (In, Ga)P layers, depth profiles of the hole concentration are displayed in Fig. 3. For the weakly ordered sample, hole accumulation and depletion are clearly observed on the GaAs and (In, Ga)P sides of the interfaces, respectively. In contrast, a remarkable hole depletion exists at the normal heterointerface with highly ordered (In, Ga)P. The hole distribution at the inverted interface of the $\eta = 0.50$ sample could not be determined, because the capacitance of the corresponding MS contact depends on the frequency. For $\eta = 0.23$, the valence-band edge in (In, Ga)P is obviously lower than in GaAs. Together with the results on n-type heterojunctions grown under similar conditions (cf. Figs. 1 and 2), it is evident that (In, Ga)P/GaAs interfaces with weakly ordered (In, Ga)P are of type I.

The two interfaces in p-type heterojunctions are again not identical. For $\eta = 0.23$, the peak of the hole density at the normal interface is lower than that at the inverted junction. By integrating the hole distributions at each interface, a deficit (excess) of holes is found at the normal (inverted) interface. With increasing η, the hole deficit at the (In, Ga)P-on-GaAs interface becomes larger and reaches for $\eta = 0.50$ values above 1×10^{12} cm^{-2}. The deficit and excess of holes are due to positive and negative sheet charges, respectively.

Comparing the carrier distributions in n- and p-type GaAs/(In, Ga)P/GaAs heterostructures, it is suggested that the deficit of the electron density and the excess of the hole density at the inverted interfaces have the same origin, i.e., negative sheet charges. Such charges lift the conduction- and valence-band edges and lead to a depletion of electrons and an accumulation of holes. At the normal interfaces, the electron surplus and the hole deficit are correspondingly caused by positive sheet charges, which lower the band edges.

For the (In, Ga)P/GaAs interfaces investigated, data are compiled in Fig. 4. Positive and negative sheet charges are

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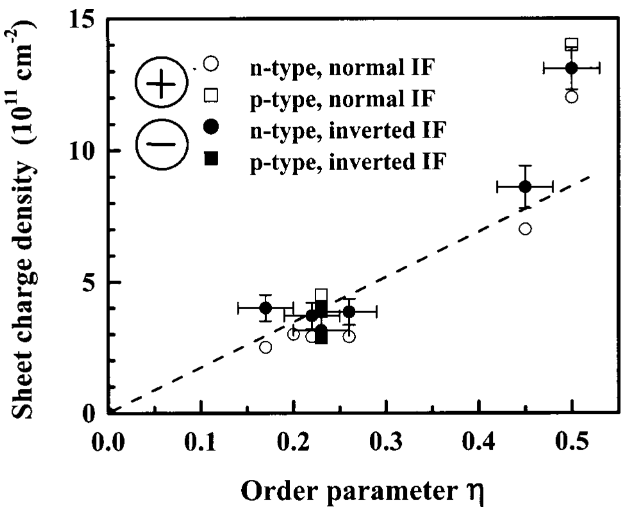

FIG. 4. Sheet charge density at normal and inverted (In, Ga)P/GaAs interfaces (IF) vs order parameter η. Closed and open symbols denote negative and positive charges, respectively. For negative sheet charges, error bars are depicted. The dashed line is a guide to the eye.

displayed as open and closed symbols. The density of all the distinct charges increases with increasing η of the (In, Ga)P layer. Positive and negative sheet charges are observed in all heterojunctions at normal and inverted interfaces, respectively. For the same sample, the absolute values of the charge densities at the normal and inverted interface are comparable, although the two interfaces are electrically screened. For (In, Ga)P with the same order parameter, the concentration of positive (negative) charges at normal (inverted) interfaces does not depend on the conduction type of the heterojunction, i.e., on the position of the Fermi level. It can be, therefore, excluded that an interfacial level in the band gap generates the same sheet charge in *n*- and *p*-type samples. Dopant atoms or deep-level defects, which might aggregate at the interfaces, can be therefore ruled out as the origin of the sheet charges.

The experimental results can be completely explained by taking into account the spontaneous polarization of ordered (In, Ga)P. In agreement with the theoretical prediction in Ref. 2, we find opposite sheet charges at the normal and inverted (In, Ga)P/GaAs interfaces due to the polarization difference between ordered (In, Ga)P and GaAs (no polarization). The explanation is further confirmed by the fact that the density of all sheet charges increases with the order parameter η. Moreover, the charge densities measured at a certain η value are comparable for all interfaces in *n*- and *p*-type heterojunctions, since the formation of polarization charges is an intrinsic property of the spontaneously ordered (In, Ga)P/GaAs interfaces and not dependent on conduction type or layer sequence.

Other authors have also found positive and negative sheet charges at normal and inverted (In, Ga)P/GaAs interfaces, respectively.[5,13,15,20] In these investigations, the opposite sheet charges at the two complementary interfaces were, however, not associated with the order-induced spontaneous polarization of (In, Ga)P.

In conclusion, polarization charges have been identified at interfaces between spontaneously ordered (In, Ga)P and GaAs. The sheet charges have remarkable consequences for the optical and electrical properties of (In, Ga)P/GaAs heterostructures. In order to measure, for example, the band discontinuities for strongly ordered (In, Ga)P, experimental methods are necessary, which are not affected by the presence of interfacial charges. The $C-V$ measurements on *n*-type (In, Ga)P-on-GaAs interfaces (see Fig. 1) permit us to determine the conduction-band offsets ΔE_C by simulations based on solutions of the Poisson equation.[6] ΔE_C is found to be about 0.20 eV. This value does not depend on the order parameter η. Contrary to the calculations,[2] the conduction-band offset is apparently not reduced by spontaneous ordering of (In, Ga)P.

Because normal and inverted interfaces exhibit opposite charges, an appropriate design becomes important for devices. Whereas the interfacial charge density depends on the order parameter η, the charge character (positive or negative) is determined by the growth sequence. Under the MOVPE growth conditions applied, free-electron (hole) densities in the 10^{12} cm^{-2} range can be achieved on the GaAs side of the normal (inverted) interfaces with ordered (In, Ga)P without doping (polarization doping). Two-dimensional electron or hole gases and high mobilities are, therefore, expected in respective field-effect transistors.

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