Ge-GaAs (110) Interface: A Self-Consistent Calculation of Interface States and Electronic Structure[a]

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Self-consistent calculations allowing electron redistribution in a wide region around a Ge-GaAs(110) interface reveal six types of interface states. The charge densities and local density of states at the interface indicate Ge-Ga bonding states in the gap (but below the valence-band maximum) and a variety of other states at lower energy. Some estimates based on these pseudopotential results give information on band-edge discontinuities and the character of bonds across a nonpolar interface.

The microscopic theory of semiconducting heterojunctions was recently approached by Frensley and Kroemer[1] with a simple potential-matching model which allows predictions of the discontinuity of the energy gap at the interface (IF). Harrison[2] has since proposed a tight-binding theory which has more microscopic justification for its predictions but does not account fully for self-consistent rearrangement of the electronic density at the IF. Baraff, Appelbaum, and Hamann[3] have reported results of a calculation on the Ge-GaAs [Ga(100)] IF which allows electronic rearrangement in a (~ 3 layer) region at the IF. These authors concentrate on gap states and the character of covalent bonds at an idealized (unfaceted) polar IF. In this Letter we present the results of a self-consistent calculation for a periodic "supercell" containing 9 Ge and 9 GaAs layers. Achievement of electronic self-consistency in a wide region allows a detailed study of the energy dispersion and spatial distribution of IF states as well as band-edge discontinuities and the character of bonds at a nonpolar interface. For the Ge-GaAs(110) IF we find find rich electronic structure which includes *six types* of IF states. We discuss the characteristics of these states and their relevance to experimentally measurable quantities.

The Ge-GaAs IF is an interesting system to study for the following reasons. Since Ga and As bracket Ge in the periodic table, the variation in atomic size and ion-core potential will be small and systematic. A direct consequence is that the lattice mismatch ($\lesssim 0.1\%$) is small and atomic disorder at the interface (misfit dislocations), which would be an added complication, is considered to be relatively small in this system. In addition many experimental results[4] are available for comparison.

The method of calculation employed in the present study has been described in detail elsewhere.[5] The ions are described by pseudopotentials which give good bulk band structures; for Ga and As the potential of Chelikowsky and Cohen[5] (CC) was used, while for Ge the potential can be characterized (in the notation of CC) by the constants $a_1 = -0.9555$ a.u., $a_2 = 0.8032$ a.u., $a_3 = -0.3121$ a.u., $a_4 = -0.018\,52$ a.u. Periodicity is artificially retained in the direction perpendicular to the IF by introducing an IF after every N (110) layers of Ge and GaAs. We have found that $N = 9$, corresponding to eighteen layers (36 atoms) in the unit cell, will give an accurate representation of the IF electronic structure (see below).

Using four k points in the irreducible part of the two-dimensional Brillouin zone, iteration[5] was continued until both the potential and the eigenvalues were stable to ~ 0.03 eV. The calculated results verify that the (110) IF remains semiconducting as expected, since for this nonpolar IF all bonds remain saturated (at least on average) and there is no energy gain to first order in any distortion. To relate the energies of IF states to the band structures of the bulk materials, the projected band structures of Ge and GaAs, calculated self-consistently from the same potentials used in the IF calculation, are presented in Fig. 1. The method used for the relative alignment of the projected band structures is presented below.

A full discussion of the IF states will be relegated to a longer paper, but the main characteristics can be seen in the projected band structure (Fig. 1). IF states can exist in the fundamental gap, below the valence band (< -11 eV), in the "stomach" gap (-2 to -6 eV), and in the "lower" gap (-7 to -10 eV). The states labeled S_1 and S_2 in Fig. 1 are s-like IF states derived from the As

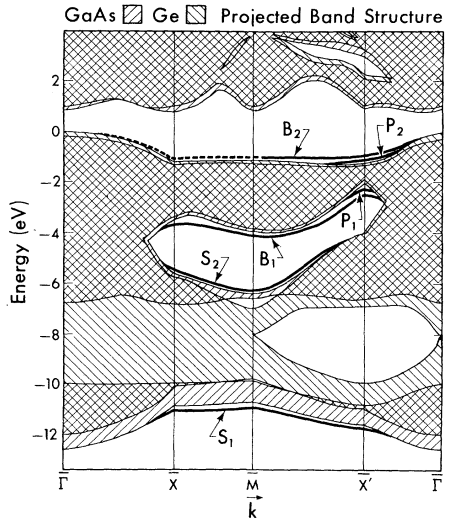

FIG. 1. The IF states of Ge-GaAs(110) relative to the projected band structures of bulk Ge and GaAs from self-consistent calculations. The dispersion of the IF states is denoted by heavy solid lines; heavy dashed lines indicate IF states which have a long decay length into the bulk. Symmetry points are $\bar{\Gamma}=(0,0)$, $\bar{X}=(\frac{1}{2},0)$, $\bar{M}=(\frac{1}{2},\frac{1}{2})$, and $\bar{X}'=(0,\frac{1}{2})$. The IF unit cell is chosen such that $a_1=a_c/\sqrt{2}$, $a_2=a_c$, where a_c is the bulk cubic lattic constant. The IF states, the "stomach" gap (−2 to −6 eV) and the "lower" gap (−7 to −10 eV) are described in the text.

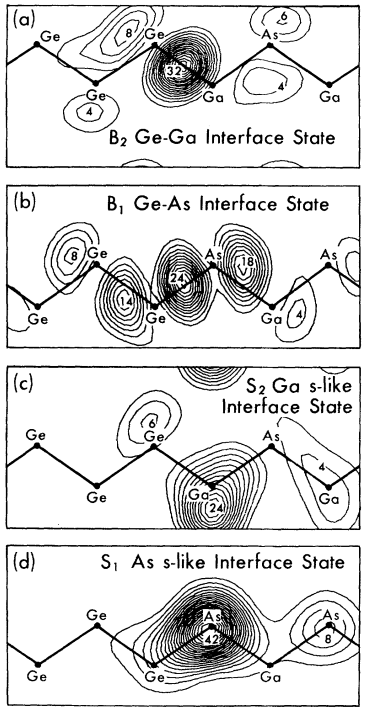

FIG. 2. Contour plots, perpendicular to the IF, of the charge densities of the IF states S_1, S_2, B_1, and B_2. Each charge density is normalized to unity over the unit cell and successive contours are separated by 2.0 units. Straight lines denote bond directions. The IF states derived from the As (respectiveity, Ga) atom are plotted in the plane containing an As (respectively, Ga) atom adjacent to the IF. In each case the charge density in the plane which is not shown is < 5% of that in the plane shown.

and Ga atoms, respectively, at the IF. Their charge densities are shown in Fig. 2. The S_2 state is not centered on the Ga atom but is displaced ~0.7 Å parallel to the IF, toward the midpoint of a line joining the two As neighbors.

States B_1 and B_2 are, respectively, Ge-As and Ge-Ga p-like bonding states directed across the IF, as is evident from the charge-denisty plots of Fig. 2. The Ge-Ga states lie in the region near the bottom of the fundamental gap and are similar to the gap states found in Ref. 3. We cannot compare directly with the results of Ref. 3, however, because of the different crystallographic IF considered. Although these are IF states in the fundamental gap, they lie below the valence-band maximum, as is clear from Fig. 1. Hence these states are not expected to show up experimentally in transport properties which sample only the band edges. The states P_1 and P_2 exist only near the symmetry point $\bar{X}'$ and are derived both from Ge-Ge and Ga-As bonds adjacent to and parallel to the IF. The lower energy state of the pair (P_1) is primarily Ga-As while the higher energy state (P_2) is mostly Ge-Ge. The charge densities of these states are much like those of bulk states at the same energy and are not shown.

The S_1, S_2 and B_1, B_2 states can be understood in straightforward physical terms. The ionic potential in the bonding region between the Ge and As atoms at the IF is stronger than that in bulk Ge or GaAs. The As-related states S_1 and B_1 respond to this and drop in energy below their bulk counterparts. Conversely the Ga-related states S_2 and B_2 are pushed higher in energy by the relatively weaker ionic potential in the Ge-Ga bonding region.

The local density of states for the Ge atomic layer at the IF is shown in Fig. 3. The high-energy part (-4 eV $< E < 0$ eV) is very much like bulk GaAs whereas the low-energy (-12 eV $< E < -4$ eV) features more strongly resemble bulk Ge. To separate the density of states localized at the IF we have compared the local density of states of Fig. 3 with those of bulk Ge and bulk

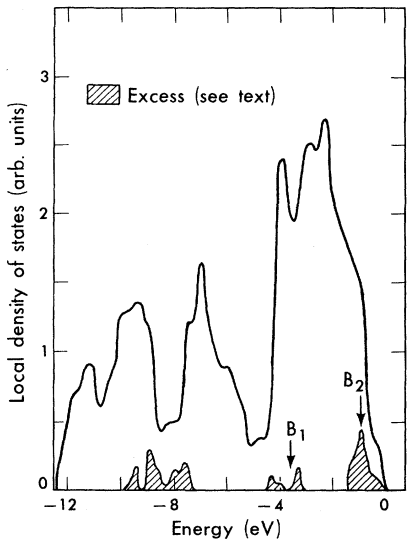

FIG. 3. The local density of states for the Ge atomic layer at the Ge-GaAs(110) interface. The "excess" denotes the density of states localized at the IF as described in the text.

GaAs. The density of states denoted as "excess" in Fig. 3 gives the energy region and amount by which the IF density of states exceeds that of either bulk. The excess features at ~ -4 and ~ -1 eV can be identified with the states B_1 and B_2, respectively, which bond across the IF layer. The states S_1 and S_2, do not lie primarily in this layer and hence do not show up in Fig. 3. There are, however, states localized at the IF in the lower gap. These are not due to true IF states but to "resonances" associated with Ge. These states surround the gap in the projected band structure (see Fig. 1) in this energy region which contains no true IF states.

We now turn to the topic of band-edge discontinuities and how the difference in energy gaps $\Delta E_g = 0.75$ eV is distributed between the valence- and conduction-band edges. This information can be obtained most accurately by first referencing the valence-band maximum to the average potential (usually fixed at zero in pseudopotential calculations) for each bulk semiconductor. Then from the IF calculation the average potential $\overline{V}^{\mathrm{Ge}}$ in Ge and $\overline{V}^{\mathrm{GaAs}}$ in GaAs can be obtained by averaging over the respective atomic layer farthest from the IF. Our calculation gives $\overline{V}^{\mathrm{Ge}} - \overline{V}^{\mathrm{GaAs}} = 0.25$ eV, of which $\lesssim 0.05$ eV is due to an electrostatic dipole. Raising the bulk energy bands of Ge by this amount results in a valence-band discontinuity $\Delta E_v = E_v^{\mathrm{Ge}} - E_v^{\mathrm{GaAs}} = 0.35$ eV, which puts a similar discontinuity $\Delta E_c = 0.40$ eV in the conduction band. We estimate our overall error to be ~ 0.1 eV. The projected band structures of Fig. 1 have been aligned in this manner, using valence-band edges and experimental gap values; the calculated gaps and conduction-band edges are not as accurate.

Experimental measurements,[4,6] however, indicate values for ΔE_c closer to 0.2 eV. If all recent measurements are given weight a value of 0.2 ± 0.15 eV is obtained. The estimates of Frensley and Kroemer[1] and of Shay, Wagner, and Phillips[7] from non-self-consistent considerations agree rather well with the experimental values, while the estimate of Harrison[2] is similar to our result. In the only previous self-consistent calculation, that of Baraff, Appelbaum, and Hamann[3] who use a method similar to that used here, it was found that $\Delta E_c \simeq -0.1$ eV (for their proposed relaxation).

Simple chemical arguments (which ignore self-consistency) would indicate that the Ge-As bond across the IF involves 9/4 electrons, 1 electron/bond from Ge and 5/4 electron/bond from As. Likewise the Ge-Ga bond would include 7/4 electrons. Such nonideal bonds as these would be weaker than Ge-Ge or Ga-As bonds, resulting in a separation of the (110) planes at the IF. This relaxation is in the direction to bring the band edges into better agreement with experiment, since for infinite separation ΔE_c is equal to the difference in electron affinities (0.06 eV).[8] When self-consistency is achieved, however, we find that charge transfer has occurred and that the total bond charge in the Ge-As and Ge-Ga bonds is 2.11 and 1.89 electrons, respectively. Thus the strength of the bonds at the IF, measured by the number of electrons that are bound, is significantly more uniform and more nearly ideal than could initially be anticipated. Study of possible relaxations at the IF is continuing. For example, the increased strength (weakening) of the Ge-As (Ge-Ga) bond could cause a tilting of the plane of the Ga-As bond.

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[1]W. R. Frensley and H. Kroemer, J. Vac. Sci. Technol. 13, 810 (1976).

[2]W. A. Harrison, to be published.

[3]G. A. Baraff, J. A. Appelbaum, and D. R. Hamann, Phys. Rev. Lett. 38, 237 (1977).

[4]A. G. Milnes and D. L. Feucht, *Heterojunctions and Metal-Semiconductor Junctions* (Academic, New York, 1972); B. L. Sharma and R. K. Purohit, *Semiconductor Heterojunctions* (Pergamon, New York, 1974). These books contain extensive lists of references on heterojunctions.

[5]J. R. Chelikowsky and M. L. Cohen, Phys. Rev. B 13, 826 (1976).

[6]R. L. Anderson, Solid State Electron. 5, 341 (1962); A. R. Riben and D. L. Feucht, Solid State Electron. 9, 1055 (1966); J. P. Donnelly and A. G. Milnes, IEEE Trans. Electron. Dev. 14, 63 (1967).

[7]J. L. Shay, S. Wagner, and J. C. Phillips, Appl. Phys. Lett. 28, 31 (1976).

[8]G. W. Gobeli and F. G. Allen, Phys. Rev. 137, A245 (1965).

Determination of the Neutron-Proton Ratio in Primary Cosmic Rays[a]

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The charge ratios of muons produced by the interaction of 400-GeV protons with thick copper targets were measured and the +/− ratios were found to be much larger than similar ratios for muons in the secondary cosmic rays. The difference between these charge ratios is taken to indicate that the neutron/proton ratio in the primary cosmic rays is quite large: i.e., of the order of 25:75.

It should be possible to derive the characteristics of secondary cosmic-ray fluxes on knowing the composition of the primary flux and the details of the hadron-hadron interactions. Conversely, the composition of the primary flux might be determined through such calculations and the results of measurements of the secondary fluxes. In this spirit, a large number of calculations have been conducted in an attempt to determine the quantitative relation between the secondary cosmic-ray muon charge ratio and the primary cosmic-ray neutron-proton ratio using information derived from high-energy accelerator experiments to describe the character of the hadron shower.

Although the calculations of the relation between the muon charge ratios and the primary composition are reasonably straightforward, some questions concerning nuclear effects and the treatment of cascades remain, and different authors have reached different conclusions.[1-3] It then seemed essential to investigate the problem experimentally by observing the charge ratios of muons produced by the interaction of high-energy nucleons with a thick target simulating the interaction of the primary cosmic-ray nucleons with the thick atmosphere. We describe here such a set of measurements, conducted at Fermilab, where we determined the charge ratio of muons of various energies produced in a thick target by the interaction of 400-GeV protons.

Secondary cosmic-ray muons are derived from the decay of mesons from hadron showers. At energies such that the probability of meson decay is smaller than the interaction probability, the character of the hadron shower would not change appreciably if the atmosphere were made uniformly denser, but the probability of meson decay would be reduced by the ratio of densities: The muon intensity would be reduced but the charge ratio would be unchanged. If the real atmosphere, with a density which varies exponentially with altitude, were replaced by an atmosphere of constant density, the relative importance of primary to secondary hadron interactions would be somewhat reduced and slightly smaller charge ratios would be observed as the charge asymmetry derived from the secondary interactions must be smaller than from primary interactions, inasmuch as charge-exchange processes act to equalize initial charge