Electronic structure of (110) Ge-GaAs superlattices and interfaces

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Ab initio energy-band calculations have been carried out for (110) Ge-GaAs superlattices containing 16 and 24 atoms per unit cell. Using the linear-combination-of-muffin-tin-orbitals method, the energy-level spectrum and local density of states were determined at selected points in the reduced zone. In agreement with earlier experimental findings, we find no evidence for well-defined localized interface states in the forbidden band.

Because of their interesting electronic and optical properties, semiconductor heterojunctions and man-made superlattices composed of alternating thin films of two different semiconductors are currently being investigated intensively.[1-5] Theories have already appeared dealing with the relative positions of the valence- and conduction-band edges on both sides of the heterojunction.[5-7] The question of the appearance of localized interface states at a given heterojunction has received relatively little attention so far.[8] If such states do occur, it would be important to understand their effects on the electronic and optical characteristics of the heterojunction or superlattice.[9]

Baraff, Appelbaum, and Hamann[8] (BAH) recently found that an ideal (100) Ge-GaAs interface gives rise to a high density of localized interface states in the forbidden band, a result in conflict with the experimental finding that there are no detectable states of this type in various Ge-GaAs heterojunctions.[10] In order to reconcile their theoretical result with experiment, BAH found it necessary to postulate a lattice relaxation or reconstruction of unknown form which removes the interface states from the forbidden band.

In this paper, we examine the electronic structure of an ideal (110) Ge-GaAs interface and demonstrate that there are no localized interface states in the forbidden band, a result that is consistent with experiment.[10] Our conclusion is not in conflict with BAH's since we are concerned with a different geometrical situation. We decided to study the nonpolar (110) Ge-GaAs interface in preference to the polar (100) and (111) interfaces because a nonpolar interface is less likely to relax or reconstruct than a polar interface. We studied Ge-GaAs because these two semiconductors have nearly identical lattice constants and so should form nearly-strain-free heterojunctions.

It is convenient to study heterojunctions by carrying out energy-band calculations for superlattices in which successive heterojunctions are reasonably well separated. We studied two different (110) Ge-GaAs superlattices, one with a repeat period of 8 layers and another with a repeat period of 12 layers. These contain 16 and 24 atoms per unit cell, respectively (Fig. 1). In these two superlattices, successive interface layers are separated by two and four bulk layers. We believe that both of these superlattices contain enough layers in the repeat period to resolve localized interface states, i.e., states concentrated on Ge-Ga or Ge-As bonds across the interface, or on Ge-Ge or Ga-As bonds within an interface layer.

The band-structure calculations for the 16- and 24-atom superlattices were carried out by the linear-combination-of-muffin-tin-orbitals (LCMTO) method[11-15] in the form described particularly in Refs. 12 and 13. Before undertaking these calculations, we used this method to determine the band structure of bulk Ge and bulk GaAs. Representing

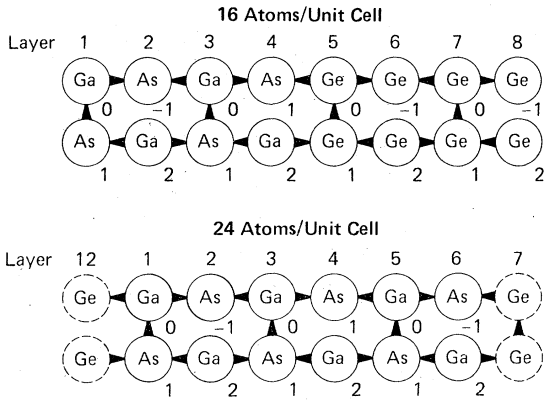

FIG. 1. Atomic arrangement of (110) Ge-GaAs superlattices with 16 and 24 atoms per unit cell. The x direction is down, the y direction is into the page, and the z direction is to the right. The y coordinates are denoted by the numbers to the right and below the atoms. In the lower figure, the bulk Ge layers are not shown but their arrangment is readily inferred.

the crystal potentials by spatial superpositions of free-atom potentials,[16] we obtained energy-band structures that are consistent with experiment and with earlier empirically refined orthogonalized-plane-wave OPW band structures.[17] As a further check, we worked out the band structure of Ge at the zone center using 16 and 24 Ge-atom-only superlattices, and verified that the results agree with the standard treatment (two atoms per unit cell).

The LCMTO method was applied to the 16 and 24 Ge-GaAs superlattices in much the same way it was applied to Si earlier.[12] There are eight basis functions (MTOs) per atom: one sp^3 set at an energy lying near the forbidden band, and another sp^3 set at an energy lying near the bottom of the valence band. The tails of the first set are damped-oscillatory, and those of the second set are damped-exponential. The superlattice potentials were represented by spatial superpositions of free-atom potentials, just as they are in standard OPW band-structure calculations.[17] The superlattices were then divided into (16 or 24) equal-volume space-filling atomic cells (Wigner-Seitz polyhedra). Each atom is thus enclosed in the atomic cell appropriate to a bulk Ge atom. The energy levels, wave functions, and orbital charge distributions were then determined at four (eight) points in the reduced zone for the 24- (16-) atom superlattice.[18] The orbital charge distributions for the various levels can be summed to obtain the local density of states (LDOS) in any particular atomic cell or any combination of atomic cells.

The total electronic density of states and the net LDOS (excess interface over bulk) are shown for the two superlattices in Fig. 2. The total DOS involves a sum over all atomic cells, while the net LDOS represents the sum over the interface cells minus the sum over an equal number of bulk cells. In the 24-atom superlattice, only the innermost bulk cells were used for generating the net LDOS. By summing the LDOS over all occupied levels, we obtain the charge content of various representative atomic cells, as indicated in Table I.

A detailed examination of the orbital charge distributions for all the levels in the vicinity of the forbidden band fails to reveal the presence of well-defined localized interface states. Such states do occur in other energy ranges, but for the most part the various superlattice levels show only a modest preference for interface or bulk atomic cells. The general situation is evident from Fig. 2, where localized interface levels can be seen near the bottom of the valence band (at about -3.1 and -3.2 Ry, for example).

Our principal results may be summarized as follows:

(a) We find no evidence for localized interface states within the forbidden band, in agreement with earlier experimental findings.[10]

(b) There is some differentiation between interface- and bulk-favored levels throughout the valence and conduction bands, as suggested by Fig. 2, but well-defined localized interface states are the exception rather than the rule.

(c) Most of the discontinuity between the GaAs and Ge valence-and conduction-band edges occurs in the lower reaches of the Ge conduction band. This was established by taking the difference between all the GaAs and all the Ge LDOS.

(d) As indicated in Table I, there is relatively little charge redistribution produced by the introduction of interfaces in the (110) Ge-GaAs superlattice. Each of the layers remains approximately electrically neutral. We believe these and other

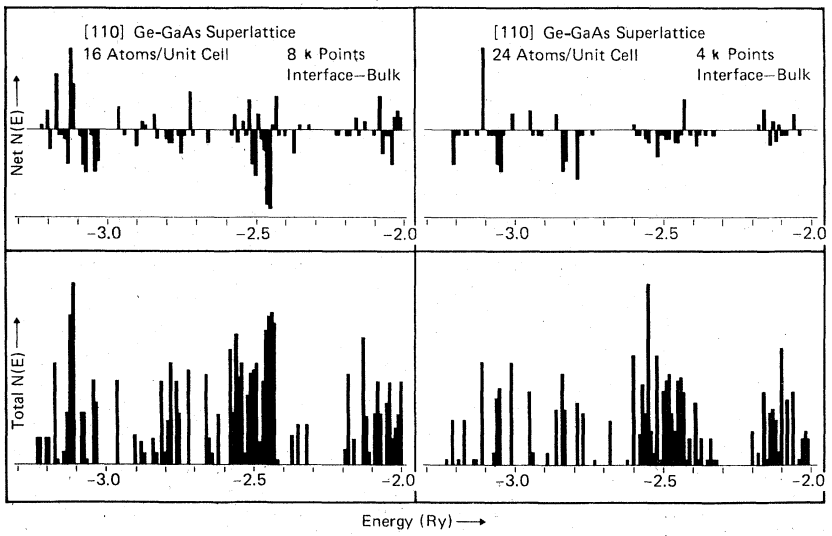

FIG. 2. Total and net local density of states for the 16- and 24-atom superlattices. The net LDOS denotes the excess of interface over bulk LDOS. The bottom of the valence band occurs at -3.23 Ry. The forbidden band lies between -2.33 and -2.25 Ry.

TABLE I. Charge content Q of representative atomic cells in 16-and 24-atom (110) Ge-GaAs superlattices. Interface and bulk atoms are distinguished by (int) and (bulk). The atoms are also identified by the indices i, j, where i denotes the layer number and j the y coordinate (as given in Fig. 1). The last two rows describe separate GaAs and Ge crystals for purposes of reference.

	Ga (int)	As (int)	Ga (bulk)	As (bulk)	Ge (int)	Ge (int)	Ge (bulk)	Ge (bulk)
16-atom superlattice								
i,j	1,0	1,1	2,2	2,−1	5,0	5,1	6,2	6,−1
Q	2.88	5.15	2.70	5.23	3.98	4.06	4.00	4.00
24-atom superlattice								
i,j	1,0	1,1	2,2	2,−1	7,0	7,1	8,2	8,−1
Q	2.78	5.25	2.58	5.38	3.93	4.06	4.00	4.00
i,j			3,0	3,1			9,0	9,1
Q			2.60	5.40			3.99	4.04
GaAs Q			2.62	5.38				
Ge Q							4.00	4.00

features of our solutions would remain the same if we were to use more sample points in the reduced zone or if we were to iterate the superlattice charge distribution to full self-consistency.

It appears, then, that the potential discontinuity across the (110) Ge-GaAs interface is not sufficiently strong to produce localized states within the forbidden band. It would be interesting to see whether such states occur when the potential discontinuity is considerably stronger, as, for example, in a (110) Ge-ZnSe heterojunction, where again the two semiconductors have nearly the same lattice constants.

Note added in proof. This problem of Ge-GaAs interface has been investigated by W. E. Pickett, S. G. Louie, M. L. Cohen, Phys. Rev. Lett. 39, 109 (1977).

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[18]Denoting the superlattice direction by z, the four k points used for the 24-atom superlattice are (000), (001), (110), and (111), in units of the Cartesian components of the reduced zone boundaries. For the 16-atom superlattice, we used these four points in the reduced zone as well as (010), (100), (011), and (101). The same charge contents were obtained for the 16 atom superlattice (cf. Table I) whether we used the first four k points, the second four k points, or all eight.