

## Electronic structure of the vacuum-semiconductor, metal-semiconductor, and semiconductor-semiconductor (111) interfaces

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A detailed study of the electronic structure of a number of (111) vacuum-semiconductor, metal-semiconductor, and semiconductor-semiconductor interfaces has been made by using a cluster-Bethe-lattice method. Numerical calculations for the electronic density of states of Ge, GaAs, and ZnSe surfaces and interfaces have been performed using a realistic Hamiltonian considering all the nearest-neighbor interactions. The results are in good agreement with those of the earlier self-consistent pseudopotential and the tight-binding calculations. A striking difference is that no true interface states (states lying in the mutual gap) are seen in the Ge-GaAs and Ge-ZnSe (111) interfaces.

### I. INTRODUCTION

Recently the use of the molecular-beam-epitaxial techniques for the fabrication of the abrupt and graded semiconductor heterojunctions<sup>1,2</sup> has spurred interest in the theoretical studies<sup>3,4</sup> of the various interfaces. A number of crystallographic interfaces like Ge-ZnSe have very important applications in technology<sup>5</sup> as transistors and photovoltaic converters. A microscopic calculation of the (100) Ge-GaAs interfaces was first made by Baraff *et al.*<sup>6</sup> A tight-binding study of the Ge-GaAs and Ge-ZnSe (100) interfaces has been made recently by Pollmann and Pantelides<sup>7</sup> using a scattering-theoretic technique. The self-consistent pseudopotential calculations have been made by Pickett *et al.* for Ge-GaAs (Ref. 8) and Ge-ZnSe (Ref. 9) (110) interfaces. In these studies attention has often been focused on the presence or absence of the interfaces lying in the gap region. In the geometry of the (110) Ge-GaAs or Ge-ZnSe heterojunctions, each atomic layer of the heteropolar semiconductor contains an equal number of the cations and anions. The surface is thus polar and both the Ge-cation and the Ge-anion bonds are broken in creating a (110) surface. The corresponding (110) interfaces with Ge are also called nonpolar and contain both the Ge-anion and Ge-cation bonds. Pickett *et al.*<sup>8,9</sup> have found these interfaces semiconducting, in agreement with the experimentally observed semiconducting (100) Ge-GaAs interfaces by Esaki *et al.*<sup>10</sup>

On the other hand, in the case of (100) GaAs or ZnSe surfaces, each layer contains only one kind of atom (cations or anions) and bonds on all the cations or anions are broken for creating a surface and the surface is polar. Two types of surfaces are thus formed, depending on the surface containing all anions or cations. For the ideal (100) interfaces, both

Baraff *et al.*,<sup>6</sup> and Pollman and Pantelides<sup>7</sup> have obtained interface states in the gap region in disagreement with the transport data of Esaki *et al.*<sup>10</sup> who have detected a semiconducting interface. To cope with this difficulty a possibility of the occurrence of the stoichiometrically mixed interfaces has been discussed.<sup>7</sup>

Some tight-binding studies of Ge-GaAs (111) interfaces have been made using either artificial<sup>11</sup> or too simple<sup>12</sup> Hamiltonians.

In the present paper we report the results of a study of the different types of the (111) interfaces of Ge, GaAs, and ZnSe by using a cluster-Bethe-lattice method. The method has successfully been employed earlier by the author for the study of the short-range order in Si-Ge alloys<sup>13</sup> and the clean and metal-covered diamond surfaces.<sup>14</sup> It has several advantages. First, one may easily solve the problem in the position space, advantageous especially with the inhomogeneous systems. Further, more often one encounters materials which are amorphous and the Bethe lattice provides a good description of the structural models for the amorphous systems rather than the crystal itself. Finally, the method is conceptually and mathematically very simple to apply and numerically easier to perform.

Although the calculations have been performed only for the (111) surfaces and interfaces, the present results should be equally applicable to the (100) and the (110) surfaces and interfaces. We will make a comparison of the results with those obtained earlier for the different geometries of the surfaces and interfaces.

The organization of the paper is as follows. A brief version of the cluster-Bethe lattice is contained in Sec. II. In Sec. III we apply the method for a calculation of the electronic density of states of the various (111) surfaces, monolayer-covered surfaces and the

interfaces of the semiconductors Ge, GaAs, and ZnSe. The results are discussed. The conclusions are contained in Sec. IV.

## II. THEORY

A Bethe lattice is an infinite nonperiodic open structure having no closed rings of interatomic bonds. For treating a local problem one may consider an appropriate cluster of atoms and attach the Bethe lattice at the cluster's surfaces, thus forming a cluster-Bethe-lattice model.<sup>15</sup> The method may easily be extended to an extended perturbation-like surface or interface. For this, one creates for each medium a two-dimensional system whose one side is kept free for a surface study or connected to a similar two-dimensional counterpart of the second medium for an interface study, while the other side is connected to the bulk medium.

In Fig. 1, two-dimensional systems appropriate to (111) surface (one for each kind of semiconductor) have been shown. We consider here a geometry where at the interface each atom of one semiconducting material is bonded to a similar atom of the second semiconducting material. All the interface bonds lie along  $\langle 111 \rangle$  or  $\langle \bar{1}\bar{1}\bar{1} \rangle$  direction. The breaking of the interface bonds creates two separate surfaces for the two materials.

We employ a nearest-neighbor tight-binding Hamiltonian where the electrons on each atom are described by one  $s$  orbital and the three  $p$  ( $p_x, p_y, p_z$ ) orbitals. One needs to know the following six interaction integrals in a material:

$$\begin{aligned} E_s &= \langle s | H | s \rangle, & E_p &= \langle p | H | p \rangle, \\ U &= \langle s | H | s' \rangle, & V &= \langle p_x | H | p'_x \rangle, \\ S &= \langle s | H | p'_x \rangle, & T &= \langle p_x | H | p'_y \rangle, \end{aligned} \quad (1)$$

where the primes on the orbitals specify the nearest-

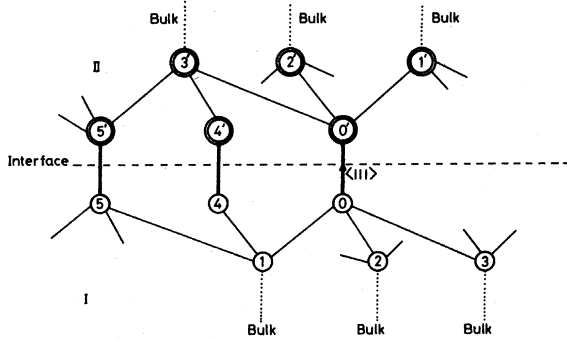


FIG. 1. Geometry of the (111) interface with the interface bonds. The two media forming the interface are denoted by I and II.

neighbor site. These integrals are considered as parameters and are fitted to the crystalline-band (especially valence-band) structure. In the bulk tetrahedrally bonded crystals, an atom has four nearest-neighbor atoms. The Green's function  $G$  is determined by the equation

$$(E\mathbf{I} - \mathbf{H}^0)\mathbf{G} = \mathbf{I} + \mathbf{V}\mathbf{G}, \quad (2)$$

where  $E$  is the electronic energy,  $\mathbf{H}^0$  is a diagonal matrix for the energies of the noninteracting  $s$  and  $p$  orbitals at an atom,  $\mathbf{V}$  is the interaction matrix between the orbitals lying on the nearest neighbors, and  $\mathbf{I}$  is the unit matrix.

Equation (2) forms an infinite set of coupled equations which, however, can be reduced to a finite set by using the symmetries of the Bethe lattice. One defines a transfer matrix or effective field  $t_{i\nu}$  at site " $i$ " for each inequivalent line joining " $i$ " to its neighbor " $\nu$ ."

The equations for the effective fields at the atoms on both sides of the interfaces are<sup>13</sup>

$$t_{10} = \left[ E\mathbf{I} - \mathbf{H}_0^i - \mathbf{V}'_{00'} t_{00'} - \sum_{j=2,3} \mathbf{V}_{0j} t_{0j} \right]^{-1} \mathbf{V}_{01}, \quad (3a)$$

$$t_{01} = \left[ E\mathbf{I} - \mathbf{H}_0^i - \mathbf{V}_{1b} t_{1b} - \sum_{j=4,5} \mathbf{V}_{1j} t_{1j} \right]^{-1} \mathbf{V}_{10}, \quad (3b)$$

$$\begin{aligned} t_{3'0'} &= \left[ E\mathbf{I} - \mathbf{H}_{0'}^i - \mathbf{V}'_{0'0} t_{0'0} \right. \\ &\quad \left. - \sum_{j=1',2'} \mathbf{V}'_{0'j} t_{0'j} \right]^{-1} \mathbf{V}'_{0'3'}, \end{aligned} \quad (4a)$$

$$\begin{aligned} t_{0'3'} &= \left[ E\mathbf{I} - \mathbf{H}_{0'}^i - \mathbf{V}'_{3'b} t_{3'b} \right. \\ &\quad \left. - \sum_{j=4',5'} \mathbf{V}'_{3'j} t_{3'j} \right]^{-1} \mathbf{V}'_{3'0'}, \end{aligned} \quad (4b)$$

$$t_{00'} = \left[ E\mathbf{I} - \mathbf{H}_{0'}^i - \sum_{j=1'} \mathbf{V}'_{0'j} t_{0'j} \right]^{-1} \mathbf{V}'_{0'0}, \quad (5a)$$

$$t_{0'0} = \left[ E\mathbf{I} - \mathbf{H}_0^i - \sum_{j=1} \mathbf{V}_{0j} t_{0j} \right]^{-1} \mathbf{V}'_{00'}. \quad (5b)$$

Here  $\mathbf{H}_0$  ( $\mathbf{H}_{0'}$ ),  $\mathbf{H}_0^i$  ( $\mathbf{H}_{0'}^i$ ) are the  $s$  and  $p$  orbital energies for the bulk and the interface atoms in semiconductor I (II), respectively;  $\mathbf{V}_{ij}$  ( $\mathbf{V}'_{ij}$ ) are the interatomic interaction matrices between the atoms  $i$  and  $j$  in the same semiconductor I (II);  $\mathbf{V}'$  are the interaction matrices for the interface bond; the subscript " $b$ " specifies the quantities in the bulk.

Equations similar to Eqs. (3) and (4) may be written down for the other effective fields at the four inequivalent atomic sites. Once these effective fields are known, the Green's function at any site " $i$ " may be written as

$$\mathbf{G}_{ii} = (E\mathbf{I} - \mathbf{H}_{ii}^0 - \mathbf{F}_{ii})^{-1},$$

with

$$E_{ii} = \sum_{j=1}^4 V_{ij} t_{ij} \quad (6)$$

The local density may then be easily obtained by

$$D_i(E) = -(1/\pi) \text{ImTr} \underline{G}_{ii} \quad (7)$$

Equations (3)–(7), along with other similar equations for the bulk semiconducting materials, can be easily solved numerically by iteration.

### III. NUMERICAL CALCULATIONS AND RESULTS

The optical gaps of the two semiconductors forming an interface are different and so are the positions of their edges of the valence and the conduction bands forming the gap. While looking for the interface states one would choose an appropriate valence-band discontinuity  $\Delta E_v$ . The conduction-band discontinuity can then easily be determined. For the (100) Ge-GaAs interface, the self-consistent pseudopotential calculation of Baraff *et al.*<sup>6</sup> has given  $\Delta E_v = 0.9$  eV. Similarly, for the (110) Ge-ZnSe interface, Pickett and Cohen's self-consistent calculation<sup>9</sup> has resulted in a value of  $\Delta E_v = 2$  eV. In view of the existing evidence<sup>16,17</sup> for a fairly small orientational dependence of  $\Delta E_v$ , it is not very crucial in assuming the above values for the discontinuities, i.e.,  $\Delta E_v = 0.9$  eV for Ge-GaAs and  $\Delta E_v = 2$  eV for Ge-ZnSe in the present calculation of the (111) surfaces and interfaces.

We will see in our later discussion that the atomic electronegativity plays an important role in determining the electron energies. In fact, on the basis of the chemical arguments, one may assign a qualitative strength to a bond between the two atoms. One way of measuring the strength of an atomic potential is its electronegativity. On this basis, for the bonds of the present interest, roughly the relative strengths of the various Ge, Ga, and As bonds as well as for the Ge, Zn, and Se bonds are  $\text{ZnGe} < \text{Ga-Ge} < \text{Ge-Ge} < \text{Ga-As} < \text{Zn-Se} < \text{Ge-As} < \text{Ge-Se}$ . In a tetrahedral configuration, the corresponding electrons per bond are 1.5, 1.75, 2.0, 2.0, 2.0, 2.25, and 2.50, respectively. In general, the location of the electron states corresponding to a chemical bond depends upon its strength, the stronger bond states appearing towards the low-energy side and vice versa.

The interaction integrals for the bulk Ge, GaAs, and ZnSe semiconductors were taken from Chadi.<sup>18</sup> The electron density has been determined for the clean Ge, GaAs (two types) surfaces, the various surfaces covered with a monolayer of the other semiconductor and the Ge-GaAs and Ge-ZnSe (each of two kinds) interfaces. We give here a discussion of each kind of system. In all the following figures the density of the bulk semiconductor has been depicted by a dashed curve.

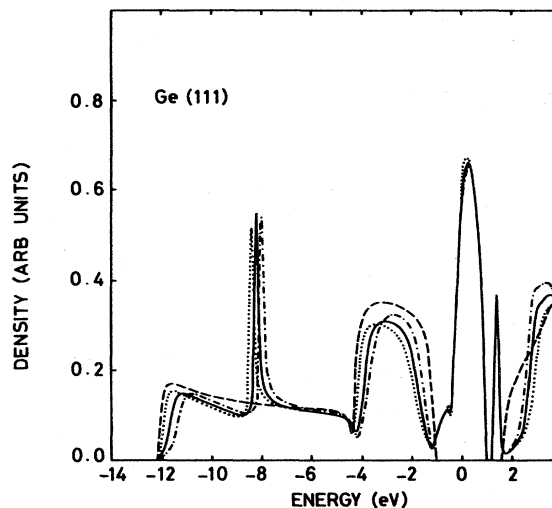


FIG. 2. Electronic states of clean Ge (111) surfaces for the different strengths of the bonds between the surface and the bulk atoms. The states corresponding to the unchanged (i.e., same as for bulk), stronger and weaker bonds are denoted by (—), (····/····), and (---) curves, respectively. The bulk density is shown by (---) curve.

#### A. Clean surfaces

*a. Ge (111) surface.* The calculated density of states for the clean Ge (111) surface is depicted in Fig. 2. In the tight-binding scheme the effect of the relaxation of the surface atomic layer can be simulated by an altered strength of the bond between the surface atom and the immediate bulk atom. Similarly the occurrence of the surface charge would result in a

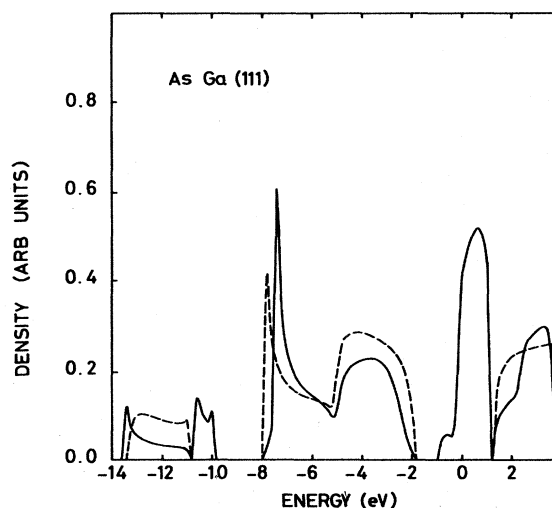


FIG. 3. The electronic density of states for the clean Ga (111) surface of GaAs is shown by the continuous curve. The states at the bulk Ga atom is shown by the dashed curve.

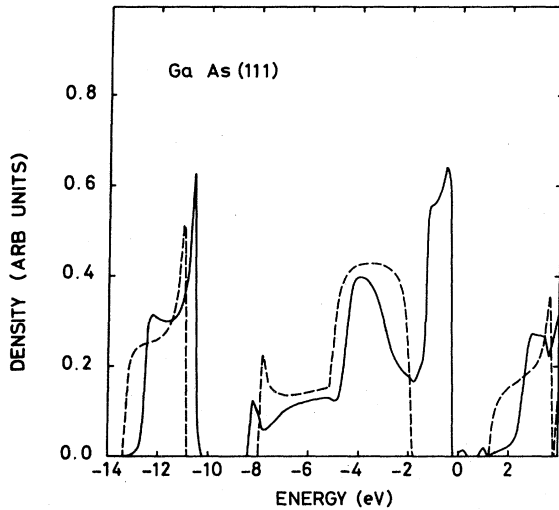


FIG. 4. Same as for Fig. 3 but for clean As (111) surface.

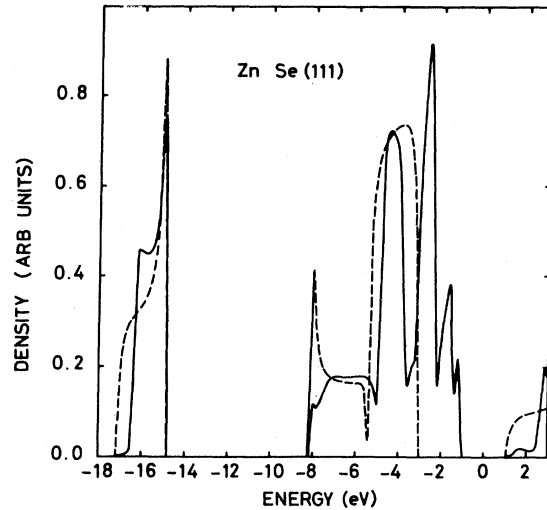


FIG. 6. Same as for Fig. 5 but for clean Se (111) surface.

renormalization of the atomic orbital energies and one may study these effects by varying the orbital energies. The effects of the variation of the strength of the bond between the surface atom and the atom lying on the layer underneath have been shown. The dangling bond *s-p*-like states appear in the gap region and a strong band of *s* states arising from the back bonds is observed in the middle of the valence band in agreement with the results of the other earlier calculations.<sup>19-21</sup> An increase in the strength of the back bond by about 10% shifts the states towards the lower-energy side, whereas the opposite is the case for a weakening of the back bond. The states in the gap are not much affected.

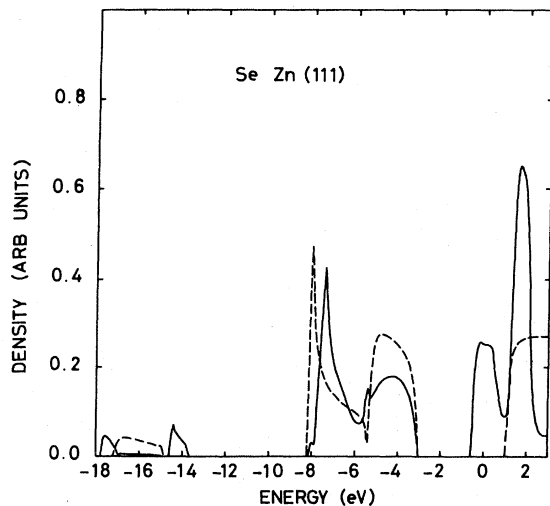


FIG. 5. The electronic states for the clean Zn (111) surface of ZnSe is denoted by the continuous curve. The bulk density at the Zn atom is shown by the dashed curve.

*b. Clean GaAs and ZnSe surfaces.* The state density for the two kinds of clean (111) surfaces of a typical III-V semiconductor GaAs and a typical II-VI semiconductor ZnSe are depicted in Figs. 3–6. There are now two different (111) surfaces for a heteropolar semiconductor as the surface may contain all cations or all anions. For comparison, in all the figures of these materials we show the local density of states in bulk at that atom which constitutes the surface layer. In Fig. 3 we note that the dangling bond states appear in the upper part of the fundamental gap because of the Ga atom being more electropositive than Ge. The Ga *s*-like back bond states peak near  $-7$  eV. Also, a weak band of the surface states appears at  $\sim -10.5$  eV, lying in the heteropolar (or “ionic”) gap. Some states occur just below the bottom of the valence band. In the case of the As surface (see Fig. 4), the dangling bond states appear towards the bottom of the thermal gap (arsenic being more electronegative). The As *s*-like states peak near  $\sim -10.5$  eV, similar to the Ga surface but with increased strength. To sum up, the states of the Ga (or As) surface are shifted to the higher (lower) side as compared to the bulk states.

In the creation of a GaAs (110), both the Ga and As bonds are broken and the resulting surface density would be given by the superposition of the surface densities of the Ga and As terminated surfaces shown in Figs. 3 and 4. However, in practice the ideal GaAs (110) is reconstructed and the two gap bands appear at the bottom and the top of the fundamental gap due to As and Ga dangling bonds becoming further split in energy, thus moving the gap states into the valence and the conduction bands leaving the gap free of surface states, in agreement with the experimental measurements. The above results are in good qualitative agreement with the earlier results<sup>3</sup>

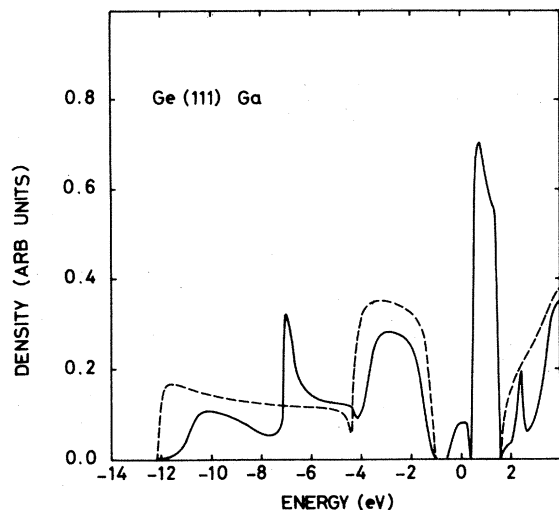


FIG. 7. The electronic states of Ga monolayer on Ge (111) surface is shown by the continuous curve. The bulk density of Ge is depicted by the dashed curve.

of the tight-binding and the pseudopotential calculations for the (100) and (110) surfaces.

The II-VI compound ZnSe is more ionic than GaAs, and one should see the effects of the increased ionicity in the surface states of these systems. The surface states of the two types of ZnSe surfaces are depicted in Figs. 5 and 6. The dangling bond gap states, due to the more (less) electronegative Se (Zn) atom compared to As (Ga) atom, appear nearer the top of the valence band or nearer the bottom of the conduction band, respectively. For Zn surfaces (Fig. 5) a few Se *s*-like surface states appear just below the valence band and there is a weak band at -14 eV in the heteropolar gap. Zn *s*-like states appear in the

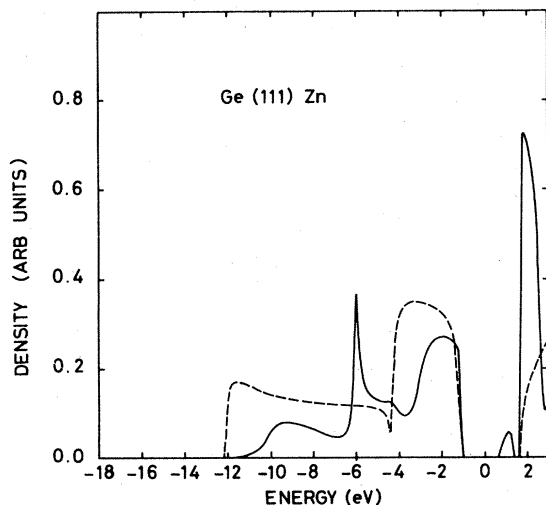


FIG. 8. Same as for Fig. 7 but for Zn monolayer.

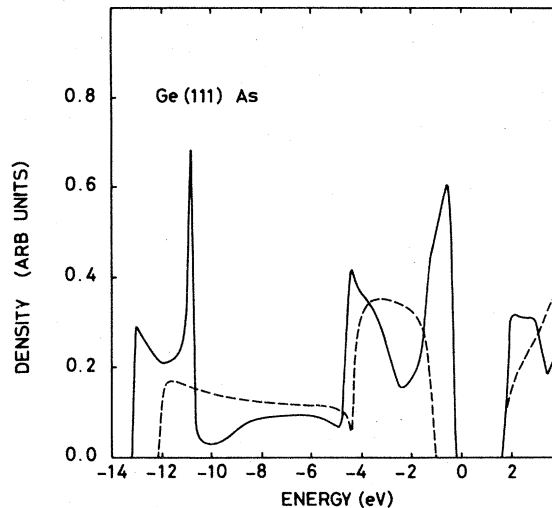


FIG. 9. Same as for Fig. 7 but for As monolayer.

energy region -5 to -7 eV. For the Se surface (Fig. 6), Se *s*-like states appear around  $\sim -16$  eV. No states appear in the heteropolar gap. In the energy region -5 to -7 eV, the surface states are now *p*-like states of Se in contrast to the *s*-like states of Zn.

The results are in agreement with those of the pseudopotential calculation of Chelikowsky and Cohen<sup>22</sup> for (110) surfaces. However, the Zn dangling bond appears well within the conduction band in their calculation in contrast to the present one lying below the conduction-band edge.

#### B. Monolayers on the Ge (111) surface

We now study the states of the anion and cation monolayers on the Ge surface. The chosen geometry

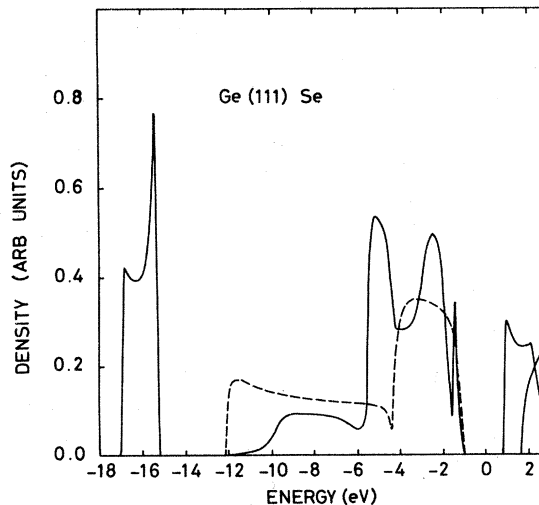


FIG. 10. Same as for Fig. 7 but for Se monolayer.

is the substitutional one, i.e., a triply coordinated one in which each adsorbate atom has its three neighbors in the Ge-substrate layer underneath. The effects of the electronegativity may be observed if we replace the surface Ge layer by an atomic layer of a different kind. This has been done for Ga, Zn, As, and Sn atoms. The interaction parameters for the Ge–Ga or Ge–As bonds have been taken as the averages of the corresponding parameters for the constituent atoms in the bulk. The results are presented in Figs. 7–10.

An atomic monolayer of Ga—cation more electropositive than Ge (Fig. 7)—has electronic states shifted towards the higher-energy side as compared to the Ge surface layer. Both the metal-induced states in the gap and the back bond states are shifted. The Ge-Ga bond states appear at  $\sim -7$  eV, in contrast to those of the Ge-Ge bond states at  $\sim -8$  eV. The Ga-monolayer also enhances the *s*-like states in the region  $-4$  to  $-7$  eV. For the monolayer of Zn (Fig. 8), which is more electropositive, similar features appear though the states are shifted more towards the higher-energy side. The Ge-Zn bond states now peak at  $\sim -6$  eV. Enhanced states are seen just at the top of the valence band. The metal-induced states now merge with the conduction band.

The electron density of the anion monolayers like As (Fig. 9) and Se (Fig. 10) show opposite trends as compared to the cation monolayers. The electron energies are shifted towards the low-energy side. The *s*-like states of As appear below the valence band and the Ge-As bond states peak near  $\sim -11$  eV. The *p*-like states appear at  $\sim -4$  eV. The gap states occur just at the top of the valence band. For the more electronegative Se monolayer (Fig. 10) the Se *s*-like

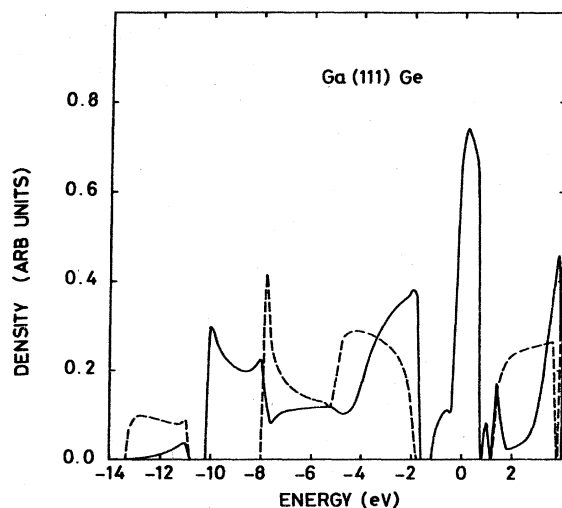


FIG. 11. The electronic density for the Ge monolayer on Ga (111) surface is denoted by the continuous curve. The density of bulk Ga atom in GaAs is shown by the dashed curve.

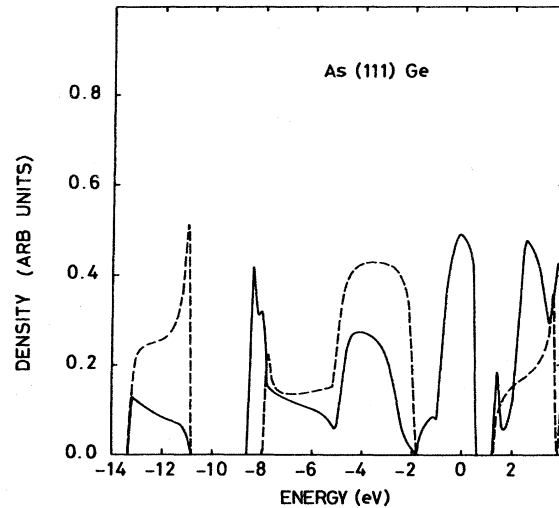


FIG. 12. Same as for Fig. 11 but for the Ge monolayer on As (111) surface.

states split from the valence band of Ge. The gap states due to quite electronegative Se are pushed into the valence band.

### C. Ge monolayers on GaAs and ZnSe surfaces

The electron states of the Ge monolayer on the cation (Ga, Zn) surfaces are shown in Figs. 11 and 12 and those on the anion (As, Se) surface in Figs. 13 and 14. All the monolayers contain the dangling bond states of Ge in the semiconductor gap. The *s*-like states of Ge lying in the lower part of its valence

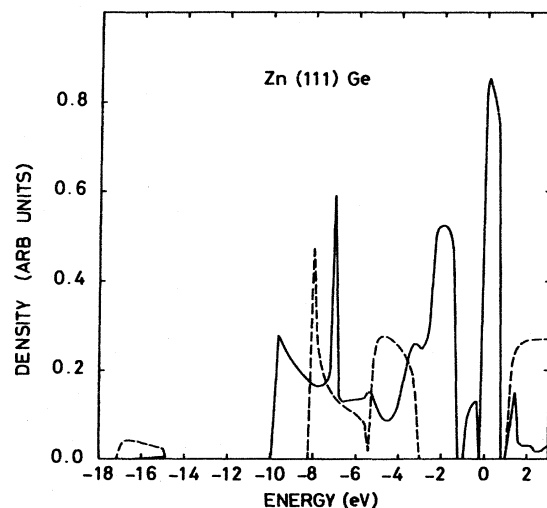


FIG. 13. The electronic density of states for the Ge monolayer on the Zn (111) surface is shown by the continuous curve. The density at the bulk Zn in ZnSe is shown by the dashed curve.

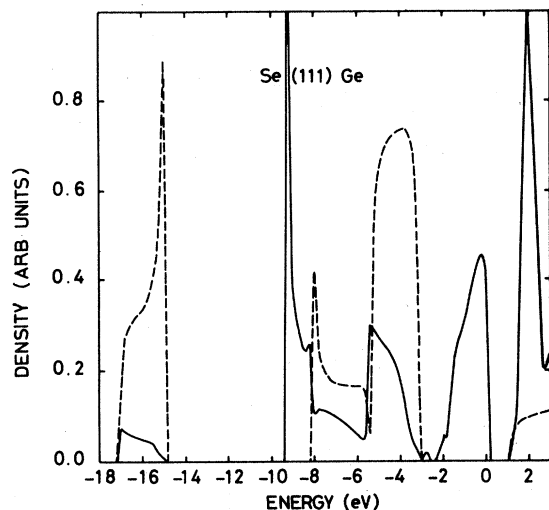


FIG. 14. Same as for Fig. 13 but for Ge monolayer on Se (111) surface.

band appear in the heteropolar gaps of the substrates GaAs and ZnSe. The states of the stronger Ga-Ge bond appear in the lower-energy side as compared to those of the weaker Zn-Ge bond. The electronic energies of the comparatively quite strong As-Ge and Se-Ge bonds, as clear from Figs. 13 and 14, appear in the low-energy region. Appreciable anion *s*-like states appear on the Ge atom on the lower-energy side of the heteropolar gap. The very strong Ge-Se bond has its states shifted to the lower-energy side.

#### D. Ge-GaAs (111) interfaces

The density of the Ga and Ge atoms at the interface formed by the Ga-Ge bond is depicted in Fig. 15, whereas the density of As and Ge atoms at the As-Ge interface is presented in Fig. 16. No interface states appear in the mutual gap, i.e., the gap region common to bulk Ge and GaAs. However, in the Ga-Ge interface, Ge *p*-like interface states appear near the top of the valence band at both the Ga and Ge atoms which decay away from the interface. A band of interface states occurs at  $\sim -9.0$  eV, strong at Ge and weak at the Ga atom at the interface (Fig. 15). This corresponds to the surface back bond band lying near  $\sim -8.0$  eV seen above in the clean Ge surface. A small density also appears near  $\sim -4.2$  eV at both the layers forming the interface.

In the As-Ge interface (Fig. 16), As *s*-like surface states appear just at the bottom of the valence band of GaAs and just below the valence band of Ge. These states decay rapidly away from the interface towards the bulk Ge. The interface band similar to the Ge-Ga interface appears approximately at the same energy ( $\sim -8.5$  eV). Some interface states also ap-

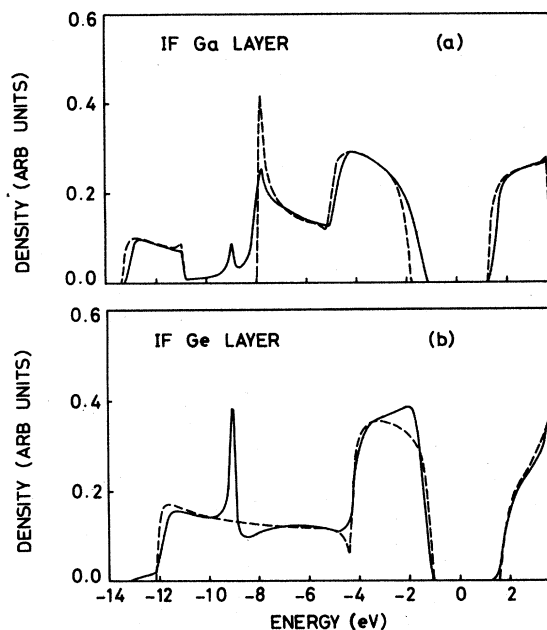


FIG. 15. The electron states of the Ge-GaAs interface. (a) The density at the Ga-interface layer is shown by the continuous curve. The density at the bulk Ga layer is shown by the dashed curve. (b) The density at the Ge-interface layer is shown by the continuous curve and at the bulk Ge layer by the dashed curve.

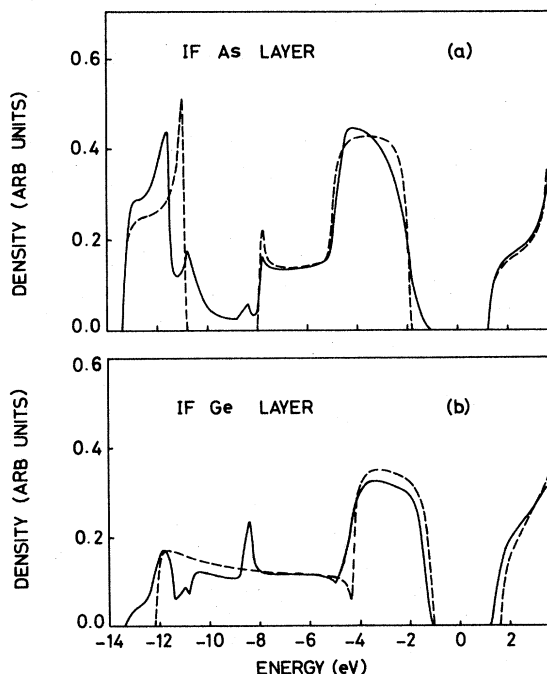


FIG. 16. Same as for Fig. 15 but for the As-interface layer.

pear near  $-4.2$  eV, similar to the Ga-Ge interface. There is a depletion of Ge  $p$ -like states near the top of the valence bands.

The above behavior of the interface states can be understood on the basis of the chemical considerations. The 3-, 4-, and 5-valence electrons of each Ga, Ge, and As atoms are distributed among the four tetrahedral bonds in a semiconductor, thus contributing 0.75, 1.0, and 1.25 electrons per bond, respectively. A Ga-Ge bond will contain only 1.75 electrons and have a deficiency of 0.25 electrons per bond, making the bond weaker. On the other hand, as an As-Ge bond will contain 2.25 electrons per bond, an excess of 0.25 electrons per bond, it will be stronger. Thus, the  $s$ - and  $p$ -like states of the weak (or strong) bond of Ge-Ga (or As) are shifted towards the higher- (or lower-) energy side compared to the bulk GaAs states and give rise to the localized interface states.

Louis<sup>11</sup> has also made a similar calculation for the Ge-GaAs (111) surfaces assuming the interatomic parameters to be the same for Ge and GaAs. His results are in agreement with the results of the present calculation.

#### E. Ge-ZnSe (111) interfaces

The state density of Ge-ZnSe interfaces are shown in Figs. 17 and 18. Although the features are similar

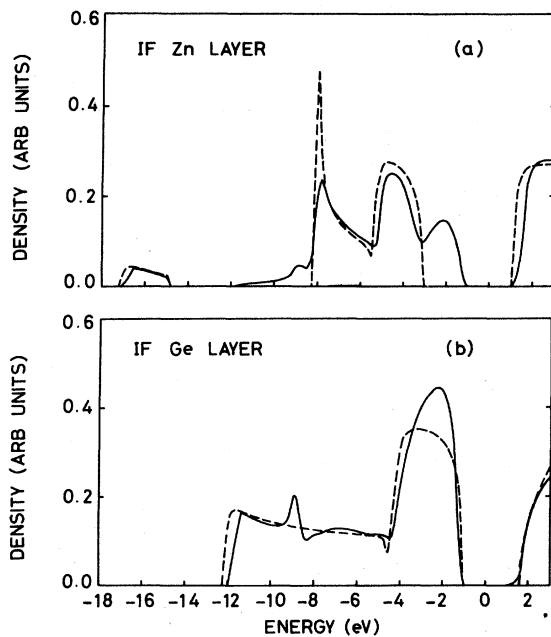


FIG. 17. The electronic density of the Ge-ZnSe interface. (a) The density at the Zn-interface layer is shown by the continuous curve. The density at the Zn layer in the bulk is shown by the dashed curve. (b) The densities at the As-interface atom and the bulk As layer are shown by the continuous and dashed curves, respectively.

to the corresponding Ge-GaAs interfaces, they are more prominent because of the large ionicity of ZnSe. Again no interface states appear at the mutual gap. For the Ge-Zn interface (Fig. 17) there is a greater density of interface states near the top of the valence bands. The band corresponding to the Ge back bond surface states is weaker and appears again near  $\sim -9$  eV. For the Ge-Se interface (Fig. 18) the Se  $s$ -like states at the Se layer appear at the bottom of the valence band of ZnSe. The Ge-interface layer has picked up a small Se  $s$ -like state which is now split from the Ge valence band. Another band, similar to the other interfaces, occurs near  $\sim -8.5$  eV. A depletion of  $p$ -like states is observed at the top of the valence band. Interface states also appear near  $-5$  eV.

#### IV. CONCLUSIONS

The above results for the interfaces are in general agreement with those of the tight-binding calculation of Pollmann and Pantelides<sup>7</sup> for the (100) Ge-GaAs and Ge-ZnSe interfaces. However, a very notable difference is that we do not see any interface states in the mutual gaps of the Ge-GaAs and Ge-ZnSe (111) interfaces as noted by them. In the creation of the

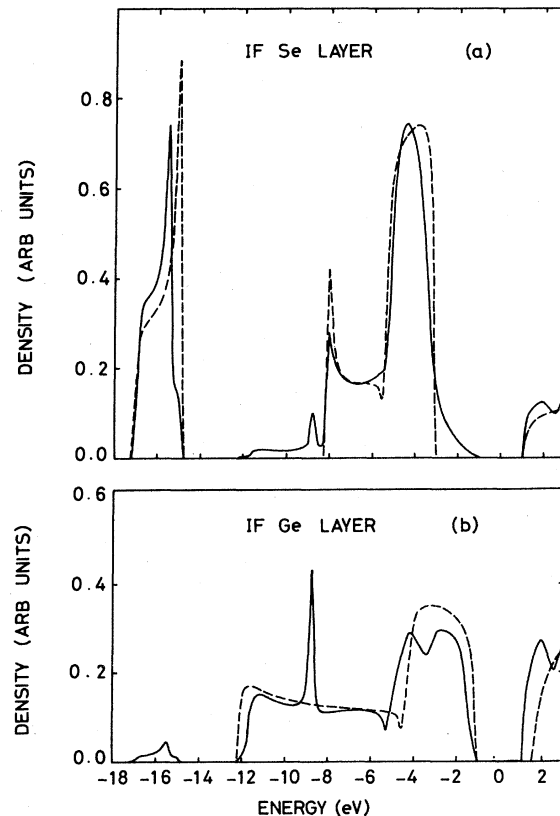


FIG. 18. Same as for Fig. 17 but for the Se atomic layers.



(100) interfaces studied by these authors, as only one kind of interface bond [Ge-Ga(Zn) or Ge-As(Se)] occurs similar to (111) interfaces, one expects similar features.

In the formation of (110) interfaces, both kinds of interface bond occur. Thus, the state density for these interfaces would be obtained by a superposition of the states corresponding to the two kinds of interface bond [e.g., a superposition of Figs. 15(a) and 16(a) for the GaAs layer and a superposition of Figs. 15(b) and 16(b) for the Ge layer for the (110) Ge-GaAs interface]. The results are in very good agree-

ment with those of the self-consistent pseudopotential calculation of Pickett and Cohen<sup>9</sup> for the (110) Ge-GaAs and Ge-ZnSe interfaces.

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