

# Geometry of the abrupt (110) Ge/GaAs interface<sup>a)</sup>

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We have studied the structure relaxation at the abrupt (110) Ge/GaAs interface by applying quantum chemical methods to clusters modeling this interface. Application of this model to bulk Ge and to bulk GaAs leads to theoretical Ge-Ge and Ga-As bond distances of 2.452 and 2.451 Å, respectively, in good agreement with the experimental values of 2.450 and 2.448 Å, respectively. Application of the model to the Ge/GaAs (110) interface indicates that this interface is nearly ideal. We find a very slight reconstruction at the interface leading to a Ge-Ga bond distance which is 0.04 Å longer than the Ge-As bond distance of 2.430 Å. The calculated spacing of the interface layer is 2.3% greater than that of bulk Ge or bulk GaAs.

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## I. INTRODUCTION

During the past few years a considerable amount of work has been directed toward understanding the formation of semiconductor-semiconductor interfaces.<sup>1-4</sup> These interfaces are of great interest due to their importance in practical semiconductor devices (heterojunctions, such as Ge/GaAs), as well as in the rapidly advancing field of superlattices (for instance, AlAs/GaAs). Most of the experimental work on interfaces has been performed on systems that require the deposition of only one component on a (compound) semiconductor substrate, such as Al, Au, or Ge on GaAs or AlAs. In this paper we will consider the (110) interface for the Ge/GaAs system, which is attractive because of the nearly perfect lattice match between Ge and GaAs. Furthermore, experiments<sup>5,6</sup> have shown that it is possible to grow epitaxially an abrupt interface by evaporating Ge on GaAs (110).

Experimentally it was found by Bauer *et al.*<sup>5</sup> and by Mönch and Gant<sup>6</sup> that the interface characteristics depend critically on the growth temperature  $T_G$ . Bauer *et al.*<sup>5</sup> find that for  $T_G \geq 450^\circ\text{C}$  the interface is broadened by diffusion, whereas for  $T_G \approx 20^\circ\text{C}$  island formation of Ge on GaAs (110) occurs. Only for a small range of growth temperatures,  $350^\circ\text{C} \leq T_G \leq 430^\circ\text{C}$ , do they observe an abrupt interface, one or two monolayers wide. They conclude that for all growth temperatures the Ge atoms bind equally to surface Ga and surface As atoms in the initial stages of interface formation. When diffusion takes place it is found that there is a preferential out diffusion of As atoms from the substrate. Similarly, Mönch and Gant<sup>6</sup> find that an abrupt interface (one to two monolayers wide) is formed for  $T_G = 295^\circ\text{C}$ , whereas for  $T_G = 395^\circ\text{C}$  the interface is broadened by diffusion. These authors conclude that in the initial stages of interface formation the Ge atoms bind preferentially to surface As atoms. Mönch and Gant find that these Ge/GaAs interfaces lead to acceptor levels that serve as electronic traps, decreasing the usefulness of such interfaces.

Theoretical work on the Ge/GaAs (110) interface has been carried out using band structure methods.<sup>7-9</sup> The disadvan-

tage of these methods is that the interface geometry must be guessed and is invariably chosen to be the ideal zincblende structure. This can lead to discrepancies between the theoretical and experimental results, due to reconstruction of the interface. Indeed, Baraff *et al.*<sup>7</sup> find the Ge/GaAs (100) interface to be metallic in this ideal geometry, whereas experimentally the interface is determined to be semiconducting. Similarly, Pickett and Cohen<sup>8</sup> conclude from charge density considerations that the Ge-Ga and Ge-As bonds are of different strength in the ideal Ge/GaAs (110) structure, which may lead to relaxation at the interface.

To obtain atomic geometries of the various interfaces that can then be used as input for band structure calculations of semiconductor-semiconductor interfaces, we have determined the atomic geometry of the abrupt (110) Ge/GaAs interface with the methods of quantum chemistry.<sup>10-12</sup> Since these methods lead to *total energies* of the systems under consideration, they are well suited for a determination of the geometries. These methods cannot at present be applied to infinite systems, so that the system under consideration must be modelled by a finite cluster of atoms. To model the Ge/GaAs (110) interface we have focused on a ring of six atoms extending across the interface (see Fig. 1). Each atom in the ring has two bonds within the ring and two bonds outside the particular ring. To represent bonds to atoms not included in the ring we have replaced those bonds by bonds to hydrogen atoms (see also Sec. II). To provide a check on the calculations this model was also applied to bulk Ge and bulk GaAs. Furthermore the model contains both Ge-Ga and Ge-As bonds, so that differences between those two types of bonds can be studied. Finally the model allows one to investigate subsurface relaxation. In Sec. II we will discuss the application of this model to bulk Ge and bulk GaAs, as well as some of the complications that occur in applying this model to bulk GaAs. This will lead to optimum models for the Ge/GaAs (110) interface, which will be discussed in Sec. III. There we give the results of the geometry optimization for the interface models. Implications of these results will be discussed in Sec. IV.

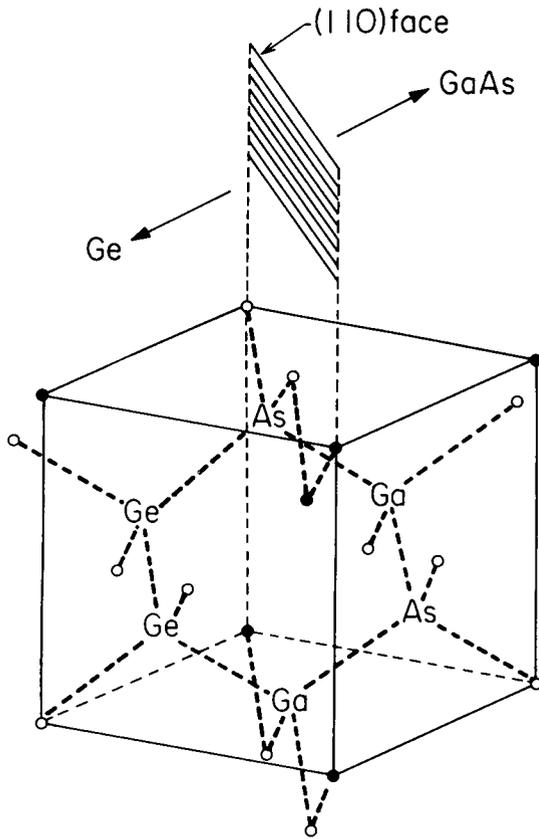


FIG. 1. Ring model for the Ge/GaAs (110) interface. The 6 atoms used in the ring are labeled. The 12 neighboring atoms are indicated by open circles.

## II. RESULTS FOR BULK Ge AND BULK GaAs

### A. Bulk Ge

The interface model outlined in the previous section can also be used to describe bulk Ge by replacing all Ga and As atoms with Ge atoms, leading to a  $\text{Ge}_6\text{H}_{12}$  model. Each ring atom will form two covalent bonds to its nearest neighbors in the ring, as well as two covalent bonds to hydrogen atoms, which represent the rest of the crystal. The hydrogen atoms are meant to mimic the effect of Ge–Ge bonds to those Ge atoms that are not included in our cluster. However, an H atom is more electronegative than a Ge atom and hence use of hydrogens may pull some charge away from the Ge's. For example, a model of bulk Ge might be to use a  $\text{Ge}(\text{GeH}_3)_4$  cluster, where the central Ge is bonded to four Ge atoms, each of which is further bonded to three H atoms (in tetrahedral positions). Use of real H atoms and a model Ge–H distance of 1.544 Å (from  $\text{GeH}_4$ ) causes the peripheral Ge atoms to lose charge to the hydrogens, while the central Ge gains an excess of 0.16 electrons (Mulliken populations). In order to let the terminal H better represent a Ge, we proceed as recently implemented by Redondo *et al.*<sup>16</sup> for Si. Placing a pseudohydrogen  $\bar{\text{H}}$ , hereafter referred to as a germanogen, at the normal position of a Ge, the electronegativity of the H atom is modified by changing the scale factor of its basis set until the charge at the central Ge of the  $\text{Ge}(\text{Ge}\bar{\text{H}}_3)_4$  cluster is neutral. This leads to a scale factor  $\zeta = 0.3612$  ( $\zeta = 1.0$  for a free H atom).<sup>17</sup>

Using this scale factor for the  $\bar{\text{H}}$  of the  $\text{Ge}_6\bar{\text{H}}_{12}$  ring model leads to an optimum Ge–Ge bond distance of 2.425 Å, which compares well with the experimental value of 2.450 Å.<sup>13–15</sup> To obtain a perfect lattice match between the models for bulk Ge and bulk GaAs (see also next subsection) the scale factor was adjusted further leading to  $\zeta = 0.4371$  and an optimum Ge–Ge bond distance of 2.452 Å.

### B. Bulk GaAs

The interface model described in Sec. I can also be applied to bulk GaAs by replacing the two Ge atoms with a Ga and an As atom. However, in this case an additional complication occurs as can be seen by considering the valence electronic structure of Ga and As. Ga, having three valence electrons, is capable of forming three covalent bonds, which leaves an empty fourth valence orbital at a Ga site. Each As atom on the other hand has a  $4s^24p^3$  valence structure and therefore can also make three covalent bonds, but this now leaves a 4s lone pair at the As sites. This means that on the average the bonds in bulk GaAs will be about  $\frac{3}{4}$  covalent in character and  $\frac{1}{4}$  donor–acceptor-like in character (with the lone pair on the As site delocalizing into the empty valence orbital on the Ga site to form the donor–acceptor bond). If in our model we use two hydrogens as nearest neighbors for each ring atom to represent bonds to atoms not present in the ring, we force the bonds between ring atoms to be 50% donor–acceptor-like in character. This is because the bonds between a ring atom and its nearest neighbor hydrogens will be covalent, leaving only the bonds between ring atoms to absorb the donor–acceptor character. Since donor–acceptor bonds are in general very weak they lead to long bond distances, and indeed, optimizing the GaAs bond distance  $d$  for the  $\text{Ga}_3\text{As}_3\text{H}_{12}$  model leads to  $d = 2.675$  Å, whereas the experimental bond distance is 2.448 Å.<sup>18</sup> Clearly, a finite cluster making the bonds between ring atoms more covalent in character must be used in order to obtain a model of bulk GaAs. Modifying the hydrogen atoms, as in the previous section for Ge, does not solve this problem since the bonds between a ring atom and its nearest neighbor hydrogens would still remain covalent.

In order to allow the bonds in the ring to have more covalent character we have modified the cluster by bonding only one H atom to each ring atom (at a tetrahedral orientation). This leaves a lone pair on the As site pointing in the direction of its missing bulk Ga (representing a donor–acceptor bond to that missing neighbor). Similarly we are now left with an empty orbital on each Ga site pointing in the direction of its missing bulk As (representing a donor–acceptor bond in that direction). This construction allows all bonds between ring atoms to be covalent. Preserving the  $C_{3v}$  symmetry of the model, there are four possible ways of constructing a  $\text{Ga}_3\text{As}_3\text{H}_6$  model, depending on the choice of the positions of the various hydrogen atoms. To label these choices we consider again the ring model with two nearest neighbor hydrogens for each ring atom (Fig. 2). Each ring atom has one bond to a nearest neighbor hydrogen which is in the “average” plane of the ring. The hydrogens representing these bonds will be called *equatorial* hydrogens,  $\text{H}_e$ . Further, each ring atom has one bond to a nearest neighbor hydrogen which is axial to the “average” plane of the ring. The hydrogens repre-

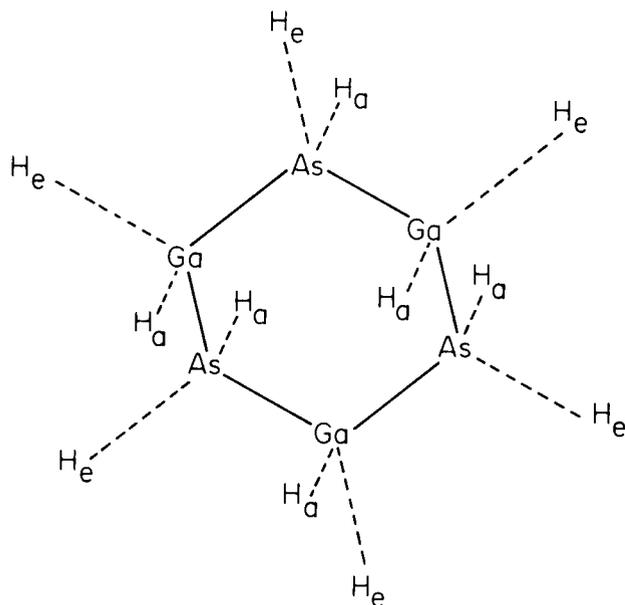


FIG. 2. Ring model for bulk GaAs, showing equatorial and axial hydrogens. With respect to a planar hexagonal ring, the three Ga's are below the plane and the three As's above the plane. The axial hydrogens are perpendicular to the plane.

senting these bonds will be called *axial* hydrogens,  $H_a$ . We now label the various models by first naming the type of hydrogen on the Ga site. This leads to the following four models: (i) equatorial–equatorial; (ii) axial–equatorial; (iii) axial–axial; and (iv) equatorial–axial.

The Ga–As bond distance  $d$  has been optimized for each of these four models and the results are given in Table I. We see that all models are now in reasonable agreement with the experimental bond distance of 2.448 Å. The small differences ( $\leq 2.8\%$ ) between the various models are not at present fully understood but are thought to be related to the space available for bonds between ring atoms in the various models. All models give bond distances slightly larger than the experimental bond distance, which is probably due to the fact that the hydrogen atoms used in these models have not been further optimized to represent bulk GaAs, but rather are just normal H atoms. The results given in Table I show that models (iii) and (iv), having axial hydrogens on the As, lead to Ga–As bond distances that are too long by 1.0% and 2.9%, respectively, which was judged to be unacceptable for modeling the abrupt interface, since the Ge–Ge and Ga–As distances must match. Models (i) and (ii), having equatorial hydrogens on the As, agree very well with experiment (error  $\leq 0.004$  Å or  $\leq 0.16\%$ ) and lead to a nearly perfect lattice match between the GaAs models and the Ge model discussed above.

TABLE I. Ga–As bond distance  $d$  for the four possible  $Ga_3As_3H_6$  models.

Model	$d(\text{Å})$
equatorial–equatorial	2.452
axial–equatorial	2.451
axial–axial	2.472
equatorial–axial	2.519

Therefore, when considering interface models, we will use models (i) and (ii) for the GaAs part.

From the results for the Ga–As bond distance given in Table I it is clear that ring models which employ only one hydrogen nearest neighbor for each ring atom give adequate results for the geometry. However, relative positions of various energy levels may be biased by the fact that there is an empty orbital on each Ga site and a lone pair on each As site. For instance, calculations of the energy difference between the ground state and the first excited state, lead to estimates for the band gap varying from 0.6 to 3.4 eV for the various models. For this reason we will consider only the geometry of the interface and make no attempt to locate various interface states with respect to the band edges. This will have to await band structure calculations that use the results of the geometry optimization as input.

### III. THE Ge/GaAs (110) INTERFACE

For the optimization of the interface geometry we have considered two models, which differ in the choice of nearest neighbor hydrogens for the Ga and As atoms. Both models consist of two Ge, two Ga, and two As atoms as in Fig. 1, but model (i) places the hydrogens on Ga and As both in the equatorial position, whereas model (ii) uses the axial position for the nearest neighbor hydrogens of the Ga atoms and the equatorial position for the nearest neighbor hydrogens of the As atoms. To determine the deviation of the interface geometry from its ideal zincblende structure, we have allowed the following relaxations of the ideal interface (bond distances to H's are not varied.):

(i) interface width ( $\Delta$ ): The width of the interface is allowed to vary, i.e., the Ge (110) surface may move away from the GaAs (110) surface over a distance  $\Delta$ :

(ii) GaAs (110) reconstruction ( $\alpha_{Ga}, \alpha_{As}$ ): The GaAs (110) surface is allowed to reconstruct in the same way as occurs on the free surface<sup>19–21</sup>; the interface Ga atom is allowed to rotate through an angle  $\alpha_{Ga}$  about the subsurface As, in the plane through the Ga atom bisecting the As–Ga–As angle in the (110) plane; similarly the interface As atom is allowed to rotate through an angle  $\alpha_{As}$  about the subsurface Ga, in the plane through the As atom bisecting the Ga–As–Ga angle in the (110) plane;

(iii) Ge (110) reconstruction ( $\alpha_{GG}, \alpha_{GA}$ ): The Ge (110) surface is allowed to reconstruct in the same way: the Ge atom bonded to a Ga atom is allowed to rotate through an angle  $\alpha_{GG}$  about its subsurface nearest neighbor, and the Ge atom bonded to an As atom is allowed to rotate through an angle  $\alpha_{GA}$  about its subsurface nearest neighbor. Positive values for the angles  $\alpha_{Ga}$ ,  $\alpha_{As}$ ,  $\alpha_{GG}$ , and  $\alpha_{GA}$  mean that the atom affected moves away from its subsurface layer, whereas negative values mean that the affected atoms move toward the subsurface layer. We have not in this study considered subsurface relaxation or alloying effects.

The results of the geometry optimizations are shown in Table II. Clearly the deviations from the ideal geometry are very small, with  $\Delta \approx 0.04$  Å and the angular distortions ( $\alpha$ ) always less than  $2^\circ$ . The two different models lead to slightly different results, which are due to the different position of the nearest neighbor H of the Ga atoms. This indicates that the

TABLE II. Deviations of the interface geometry from the ideal zincblende structure.  $\Delta$  is the increase in the width of the interface;  $\alpha_{\text{Ga}}$ ,  $\alpha_{\text{As}}$ ,  $\alpha_{\text{GG}}$ , and  $\alpha_{\text{GA}}$  are the angles through which the interface Ga, As, Ge bonded to Ga, and Ge bonded to As rotate about their subsurface atoms, respectively.

	Model 1 <sup>a)</sup>	Model 2 <sup>b)</sup>
$\Delta$ (Å)	0.046	0.017
$\alpha_{\text{Ga}}$	-0.1°	0.0°
$\alpha_{\text{As}}$	1.8°	-1.0°
$\alpha_{\text{GG}}$	0.7°	-0.2°
$\alpha_{\text{GA}}$	-0.3°	1.4°

a) The GaAs part of Model 1 is equatorial-equatorial. In the ideal structure the bond distances are chosen to be 2.452 Å.

b) The GaAs part of Model 2 is axial-equatorial. In the ideal structure the bond distances are chosen to be 2.451 Å.

use of only one nearest neighbor H atom for each Ga and each As leads to inaccuracies in the final geometry. For that reason the results given here should not be viewed as giving accurate geometries for the interface, but rather as providing trends in the interfacial relaxation. These trends can be obtained because the two models lead to similar changes in the interface geometries as can be seen more clearly from Table III. In this table we have translated the results into quantities that better characterize the interface, namely,

- (i) The Ge-Ga and Ge-As bond distances, as well as the difference between them (best value  $0.036 \pm 0.01$  Å);
- (ii) the surface strain  $\Delta(\text{Ga-As})$  of the GaAs (110) surface, which is defined as the displacement of a surface As with respect to a surface Ga, measured normal to the unreconstructed surface (best value  $0.05 \pm 0.04$  Å);
- (iii) the surface strain  $\Delta(\text{Ge})$  for the Ge (110) surface (best value  $0.02 \pm 0.03$  Å);
- (iv) the angles between the various interface atoms;
- (v) the average angles  $\gamma_{\text{Ga}}$  and  $\gamma_{\text{As}}$  about the interface Ga and As atoms, extended to their nearest neighbor As and Ga atoms, respectively.

When possible these quantities are compared to the corresponding quantities for the free GaAs (110) surface. From the results given in Table III we see that for both models the

TABLE III. Characterization of the Ge/GaAs (110) interface.  $\Delta(\text{Ga-As})$  is the surface strain for GaAs (110).  $\Delta(\text{Ge})$  is the surface strain for Ge (110).  $\gamma_{\text{Ga}}$  and  $\gamma_{\text{As}}$  are the average bond angles of the interface Ga and As atoms to their nearest neighbor As or Ga atoms, respectively.

	Model 1	Model 2	Free GaAs (110)
Ge-Ga (Å)	2.466	2.473	
Ge-As (Å)	2.430	2.448	
$R_{\text{Ge-Ga}} - R_{\text{Ge-As}}$ (Å)	0.036	0.025	
$\Delta(\text{Ga-As})$ (Å)	0.05	-0.03	0.67
$\Delta(\text{Ge})$ (Å)	0.02	-0.04	
$\angle \text{As-Ge-Ge}^{\text{a}}$	108.5	110.5°	
$\angle \text{Ga-Ge-Ge}^{\text{a}}$	109.7	109.0°	
$\angle \text{Ga-As-Ge}^{\text{a}}$	112.5	109.9°	
$\angle \text{As-Ga-Ge}^{\text{a}}$	110.2	109.6°	
$\gamma_{\text{Ga}}$	109.7	109.4°	119.5°
$\gamma_{\text{As}}$	107.8	110.4°	94.9°

<sup>a)</sup> Underlined atoms in these angles are interface atoms.

Ge-Ga distance is slightly larger than the Ge-As distance, in agreement with the fact that an As atom is slightly smaller than a Ga atom. Furthermore we see that the buckling of the surfaces as expressed by  $\Delta(\text{GaAs})$  and  $\Delta(\text{Ge})$  is very small [ $\Delta(\text{GaAs}) \leq 0.05$  Å and  $\Delta(\text{Ge}) \lesssim 0.04$  Å, whereas for the free GaAs (110) surface we have  $\Delta(\text{GaAs}) = 0.67$  Å].<sup>21</sup> All the bond angles are very close to the tetrahedral value. These results indicate that the abrupt (110) Ge/GaAs interface is nearly perfect. The following trends are observed: (1) The width of the interface increases slightly (0.02–0.05 Å), (2) The Ge-Ga bond distance is slightly longer (0.04 Å) than the Ge-As bond distance. This does not mean that the perfect abrupt interface will be easy to fabricate and indeed our analysis of the wave functions (next section) suggests that normal fabrication techniques may systematically lead to electron traps at these interfaces.

#### IV. DISCUSSION

As shown in the previous section, the results of the geometry optimization for abrupt (110) Ge/GaAs interfaces indicate that the interface has a nearly perfect zincblende structure, the most notable deviation being a small difference (<1.5%) in the Ge-Ga and the Ge-As bond distances. However, while this interface is nearly perfect it may be difficult to form. The perfect GaAs (110) surface undergoes a substantial reconstruction in which the surface As moves outward, developing a lone pair to accommodate its five valence electrons and the surface Ga moves inward to form three bonds to accommodate its three valence electrons. This reconstruction is quite large [ $\Delta(\text{Ga-As}) = 0.67$  Å] and results in a lowering of the energy per GaAs pair of 1.3 eV. To initiate the formation of the interface this barrier must be overcome. In addition even at the tetrahedral geometry of the surface of GaAs (1.3 eV uphill) the electrons are in the wrong place to bond to the Ge in forming the abrupt interface. There is still one extra electron on the As (a lone pair) and an empty orbital on the Ga. Considerations of the processes involved in bonding Ge to the surface indicate that a substantial number of defects may result in forming the interface. (Indeed there is evidence that a number of acceptor states are present at the interface.)<sup>5,6</sup>

In contrast, growth of III-V interfaces such as those between GaAs and AlAs may be much easier simply because of the similarity in the chemistry of the two constituents making up the interface. In that case bonding of As atoms to surface Ga and Al atoms to surface As would naturally provide the electrons needed for new covalent bonds without the necessity for an electron transfer process.

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