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Electronic structure of Ge and diamond Schottky barriers

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The electronic structure of metal-semiconductor (or insulator) interfaces is studied using the self-consistent pseudopotential method. The metal is simulated by a jellium model for the positive background with a charge density equivalent to that of aluminum. For the metal-Ge(111) interface, a high density of metal-induced gap states is found which pins the Fermi level. These states are free-electron-like in the jellium and decay exponentially into the Ge. The calculated Schottky-barrier height is 0.55 eV and the index of interface behavior S is 0.14, in agreement with experiment. The behavior of the diamond Schottky barrier is crucial in the theory of Schottky barriers because of its large gap and zero ionicity. For the metal-diamond interface, the density of metal-induced gap states is found to be smaller than in the case of Ge. Predictions based on experimental extrapolations give $S = 0$. Our calculations give $S = 0.4$. We obtained a barrier height of 2.2 eV, in agreement with experiment. The theory of the Schottky barrier is discussed using present results.

I. INTRODUCTION

The self-consistent pseudopotential method which has proved very successful for calculations of metal-Si and metal–zinc-blende semiconductor interfaces[1,2] has been applied to similar calculations of metal-Ge and metal-diamond interfaces. Current interest in metal-semiconductor (M-S) interfaces has focused on the dependence of the barrier height on ionicity (or gap size) of the semiconductor and the electronegativity of the metal. The central problem is the interface index S of the semiconductors which characterizes the behavior of the Schottky barrier. Some researchers have claimed that it is a crucial indicator of the covalent-ionic transition among various semiconductors.[3] The physical understanding of these properties is of continued interest and many questions still remain open.

Hopefully a theory of Schottky barriers should be able to explain the behavior of Schottky barriers of both covalent materials and ionic materials. Self-consistent pseudopotential calculations for the Schottky barriers of Si and zinc-blende materials yielded information on the local density of states, barrier heights, charge densities, interface states, and metal-induced gap states. The present paper on Ge and diamond is a complement to the previous calculations; the calculation of the diamond Schottky barrier[4] is of special theoretical importance because different theories predict different behavior for this large-gap but zero-ionicity material.[5]

The model presented here for the calculation of the electronic structure of the M-S interface is considered to be a realistic one in that the conduction electrons of the metal and the valence electrons of the semiconductor are free to redistribute self-consistently for a given system. Our model for an ideal M-S interface consists of jellium in contact with a semiconductor described in the pseudopotential formalism. There is experimental evidence for chemical-bond formation for many M-S interfaces under favorable conditions.[6] The jellium model is certainly not able to adequately describe the M-S chemical bond. We will show, however, that without taking into account the details of the chemical bond, our calculations are still in good agreement with experiment wherever experimental data are available, and this model even allows us to explain fundamental features of the behavior of the Schottky barrier in terms of metal-induced gap states (MIGS). In this sense, the jellium model serves a good starting point for a completely realistic interface calculation. In addition, a recent pseudopotential calculation of an aluminum *monolayer* on Si,[7] where the chemical bond is allowed to form, shows states in the gap which are similar to our MIGS.

The plan of the remainder of the paper is as follows: in Sec. II the calculational procedure is described. The results of the calculations are presented in Sec. III. The theory of the Schottky barrier is developed in Sec. IV. Finally in Sec. V some discussion and concluding remarks are given.

II. CALCULATIONS

Our model for an ideal M-S interface consists of jellium in intimate contact with a semiconductor described in the pseudopotential formalism. This model for the M-S interface and the method we used to calculate the interface electronic structure have been discussed in detail in Ref. 1. Hence, in this section, we shall only briefly describe some of the essential features of the method.

Two crucial features of our method are (i) self-consistency in the potential of the valence electrons is imposed to allow for the correct electronic screening near the interface and (ii) periodicity is artificially retained along the direction perpendicular to the interface to allow for the use of the usual pseudopotential techniques.

Our elongated unit cell consists of m atomic layers of the semiconductor and n layers of equivalent thickness of jellium metal. The numbers used here are $m=12$, $n=12$ for Ge metal and $m=12$, $n=20$ for diamond metal. The ratio of m to n is approximately the ratio of the Gibbs oscillation wavelength of the semiconductor valence charge density to that of aluminum charge density. These numbers are big enough to suppress significant interactions between the neighboring interfaces.

There are no adjustable parameters in the calculations. The only input consists of the structures (i.e., the geometry of the interface) and the ionic pseudopotentials of the semiconductor ion cores which are determined from atomic spectra. Present experimental and theoretical methods do not enable us to unambiguously determine the geometry at the interface. In the jellium model we are not concerned about the exact positions of the metal atoms; the single quantity to be determined for the metal is the position of the jellium edge. The edge has been taken to lie at half the semiconductor-semiconductor bond length away from the interface atom of the semiconductor. Previous calculations for the metal-Si interface showed that the interface properties are not sensitive to 25% change in this value. Semiconductor atoms are assumed to be at the ideal positions. The ionic core potential for Ge is a local pseudopotential whose Fourier transform is of the form

$$V^{\mathrm{Ge}}_{\mathrm{ion}}(q) = (a_1/q^2)[\cos(a_2 q) + a_3]\, e^{a_4 q^4} . \tag{1}$$

The same potential was used in the Ge surface calculation before.[8] For the ionic core potential of diamond, we used angular-momentum-dependent nonlocal pseudopotentials derived elsewhere.[8]

$$V_l^{\mathrm{diamond}}(r) = \frac{-8}{r + a_1 e^{-a_2 r}} - a_3 e^{[-a_4 (r-a_5)^2]} , \quad l = 0, 1 . \tag{2}$$

Parameters are found in Table I.

Screening is achieved using a Hartree potential via Poisson's equation and Slater's statistical exchange potential. We used $\alpha = 0.794$ for the local exchange potential to be consistent with previous surface calculations for Ge and diamond.[8] In addition to ionic core potentials, a starting empirical potential is needed to initiate the self-consistent loop. An adequate choice of the starting potential reduces the number of iterations required to achieve self-consistency. Details of the method are found in Ref. 1. The electronic wave function is expanded in a basis set of ~200 plane waves for the Ge Schottky barrier. Another 400 plane waves are included through a second-order perturbation scheme. Those numbers for diamond are 600 and 800, respectively. This set of plane waves gives roughly the same degree of convergence as for the previous surface calculations.

III. RESULTS

In this section, the electronic structure of the Ge-jellium and the diamond-jellium interfaces are presented. Some of the results have been briefly reported previously.[4] The results for the Ge-jellium interface are presented first. The total valence charge density is a good indicator of the quality of the present work. For the repeated slab geometry employed in our model to adequately represent noninteracting interfaces, the charge densities away from the interface should reproduce the bulk densities of the two materials. Figure 1 displays the total valence charge density in a $(1\bar{1}0)$ plane perpendicular to the interface. A few angstroms away from the interface, the charge density is essentially a constant corresponding to bulk aluminum on the metal side and bulk Ge on the semiconductor side (obtained in Ref. 8 with the same cutoff energies in the basis set), respectively. As the behavior of the Schottky barrier is determined by the states available in the gap, we will investigate these states in detail. The charge density of the gap states is plotted in the $(1\bar{1}0)$ plane perpendicular to the interface in

TABLE I. Parameters entering Eqs. (1) and (2) to define the ionic pseudopotentials of Ge and diamond. The potentials are in rydbergs and the lengths are in Bohr radii. Normalization for Ge is per bulk unit cell.

	$V^{\mathrm{Ge}}_{\mathrm{ion}}$	V^{diamond}_0	V^{diamond}_1
a_1	−0.955 46	100	9
a_2	0.803 23	5.68	4.41
a_3	−0.312 05	3	11.6
a_4	−0.018 52	1.5	1.3
a_5		0.4	−0.15

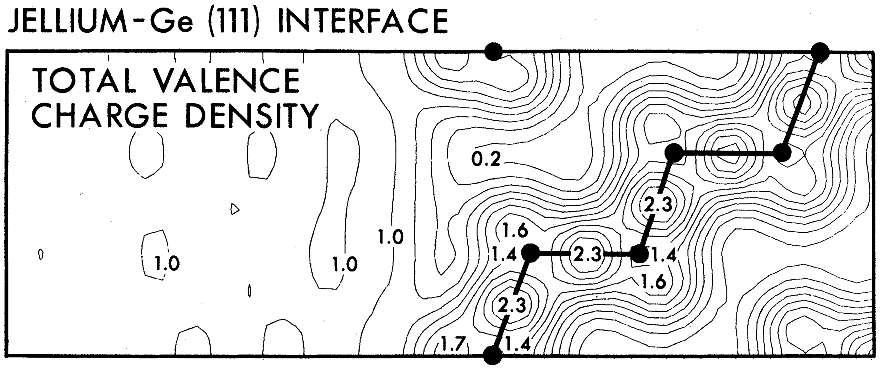

FIG. 1. Total valence charge-density contours of the jellium-Ge(111) interface in a (1$\bar{1}$0) plane. Normalization corresponds to the number of electrons per unit "supercell." The numbers in the plot should be multiplied by 8.112 to get the normalization per unit cell of bulk Ge. Therefore, the density at the bonding site is ~ 19, in agreement with 19–20 of the bulk Ge in Ref. 8. In the jellium region a typical value of 1.03 corresponds to $r_s = 2.08$, which is again in agreement with the aluminum charge density, $r_s = 2.07$.

Fig. 2(a). The same charge-density profile, $\bar{\rho}(z)$, averaged parallel to the interface and plotted perpendicular to it, is shown in Fig. 2(b). These gap states induced by metal are free-electron-like on the metal side and decay exponentially into the Ge region. The decay length δ is determined to be ~2.7 Å from Fig. 2(b), which is a little longer than the Ge-Ge bond length ~2.5 Å. There is an oscillation of the average charge in the exponential tail due to the semiconductor bond. Right at the interface these states look like dangling-bond states found in the clean Ge(111) interface.[8] Another characteristic feature of the gap states which is relevant to the behavior of the Schottky barrier is the surface density of states $D_s(E)$. For energies over the semiconduc-

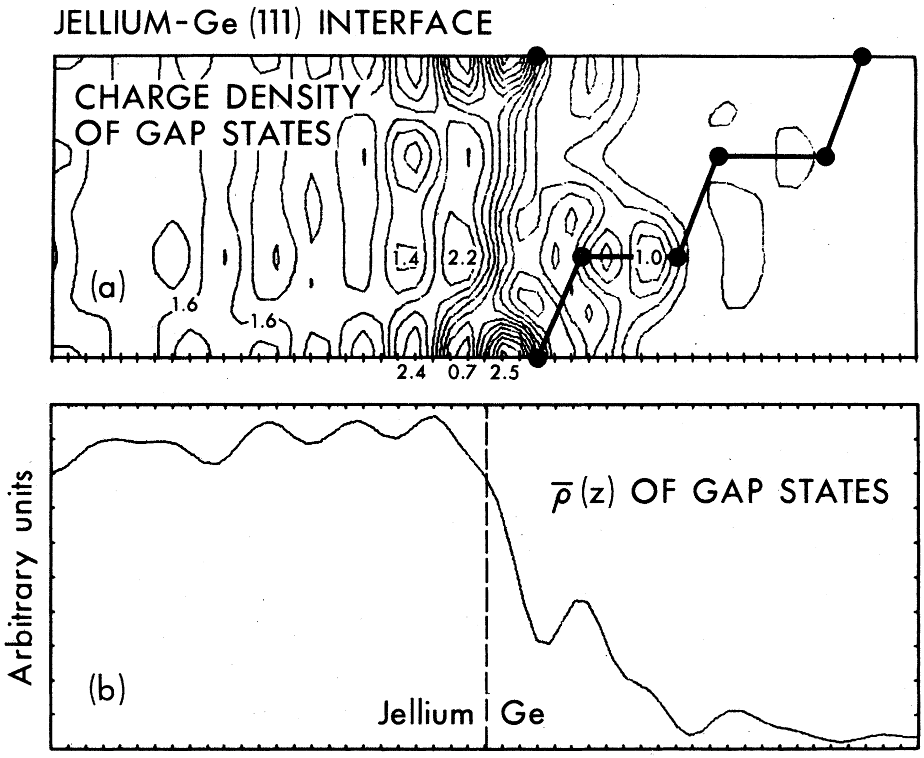

FIG. 2. (a) Charge-density contours for gap states ($0 < E < E_g$) in a (1$\bar{1}$0) plane. The numbers should be multiplied by 0.57 to get the number of electrons per unit cell of bulk Ge. (b) The same charge density averaged parallel to the interface and plotted perpendicular to it.

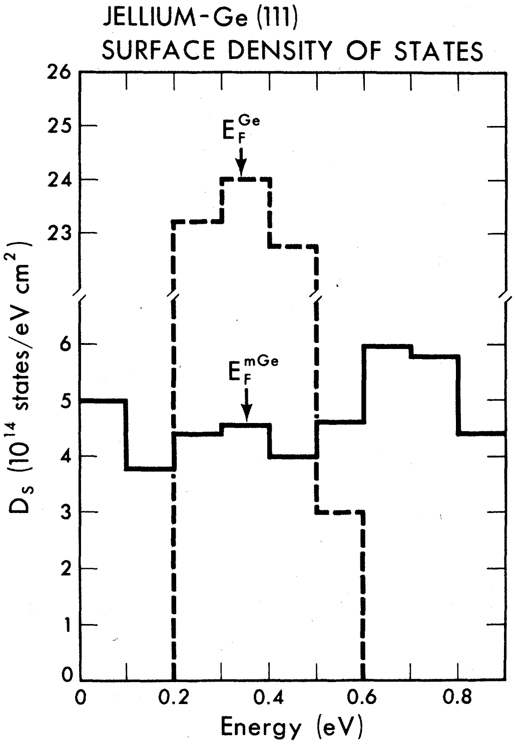

FIG. 3. Surface density of states D_s of the jellium-Ge(111) interface in the gap. Also shown (in heavy dashed lines), is the density of states of the clean Ge(111) surface states in the gap from Ref. 8. It is clear from the figure that the surface-state peak of the clean Ge is drastically reduced by the metal contact. The new metal-induced gap states give the more or less uniform D_s. E_F^{mGe} and E_F^{Ge} are the Fermi levels of the metal-Ge interface and the clean Ge surface, respectively. (Note: The density of states of the clean surface should be multiplied by the spin degeneracy 2 because it has been omitted in Ref. 8. The same is true for Fig. 6.)

tor thermal gap, we define

$$D_s(E) \equiv a^{-1} \int_a \int_0^\infty N(E, \vec{r})\, dz\, da, \quad 0 < E < E_g, \tag{3}$$

where a is the interface area, E_g is the gap, and the integral over z is to be performed from the interface to a point deep into the semiconductor bulk. $N(E, \vec{r})$ is the local density of states defined by

$$N(E, \vec{r}) \equiv \sum_{n, \vec{k}} |\psi_{n\vec{k}}(\vec{r})|^2 \delta(E - E_n(\vec{k})) . \tag{4}$$

Thus $-eD_s(E)$ gives the density of surface charge per unit energy per unit area. The calculated $D_s(E)$ shown in Fig. 3 is more or less uniform in the thermal gap region. Also superimposed in the figure is the density of states of the clean Ge(111) surface in the gap from Ref. 8. This figure clearly shows that the sharp peak of the dangling-bond states found in the clean Ge surface is dramatically reduced by the metal contact. This is an unequivocal illustration that the gap states of the Schottky barrier are not the intrinsic surface states[6,9] but the metal-derived states.[10] This is also in agreement with recent experiments.[11] The Fermi level is not shifted by the metal contact within our calculational accuracy. The calculated height ϕ_b defined to be the difference between the conduction-band minimum and the Fermi level (for the n-type semiconductor) is 0.55 ± 0.1 eV. The effect of the image force on the barrier height is neglected here. Our calculated gap of ~0.9 eV is somewhat larger than the zero-temperature thermal gap, 0.75 eV. If we should include spin-orbit splitting at the triply degenerate valence band maximum in our calculation, the top of the valence band would be raised by 0.1 eV. So our calculated gap size is in reasonably good agreement with experiment. In any case the value of ϕ_b for the n-type Ge is not affected. This value is in good agreement with the experimental values for the Ge-Al Schottky barrier ranging from 0.49 to 0.61 eV.[12,13] As electrons in our model do not experience the details of the actual Al potential, one should not attach too much significance to high accuracy. However, because ϕ_b is found almost independent of the metals in contact for the Ge Schottky barrier, this agreement is a successful aspect of our calculation. Experiments also show that the temperature dependence of the barrier height is fairly small up to room temperature, so that zero-temperature band calculation is to be compared directly with experiment.[13]

The results for the jellium-diamond interface are presented in Figs. 4–6, in the same manner as above. In Fig. 4 the total valence charge density on the metal side away from the interface region is again a constant corresponding to aluminum charge density and that on the diamond side agrees with bulk diamond calculated in Ref. 8. The average charge density of gap states plotted in Fig. 5(b) shows one noticeable difference compared to Fig. 2(b) for the Ge-jellium interface. The dangling bond of the diamond is so strong that it gives rise to depletion of charge on each side of the dangling-bond region. This effect is strongly enhanced by the fact that the number density of surface atoms of diamond is ~2.5 times as high as that of Ge. Otherwise, the overall charge distributions resemble each other. δ is 1.37 Å in this case, a little smaller than the C-C bond length ~1.55 Å. The plot of the surface density of states together with the corresponding density of states of the clean diamond surface (Fig. 6) illustrates

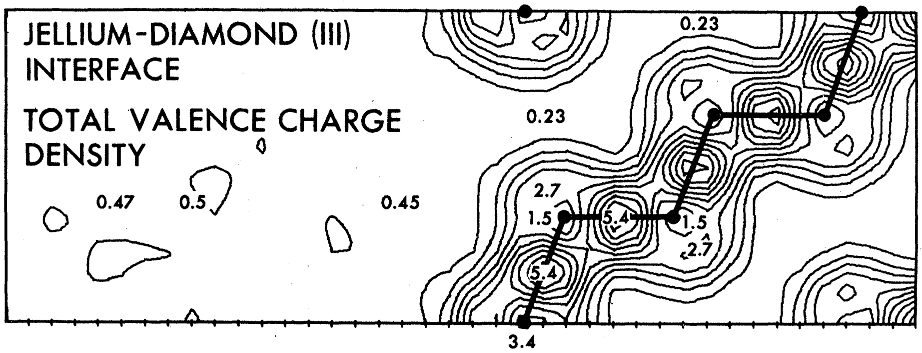

FIG. 4. Total valence charge-density contours of the jellium-diamond (111) interface in a $(1\bar{1}0)$ plane. Normalization corresponds to the number of electrons per unit "supercell," and we should multiply by 4.333 to get the normalization per unit cell of bulk diamond. Therefore, the density at the bonding site is 23.4 in agreement with 23.8 of the bulk diamond in Ref. 8. A typical value of 0.47 in the metal region corresponds to $r_s = 2.08$ in agreement with $r_s = 2.07$ of Al.

that even a more drastic reduction in the density of the dangling-bond states takes place because of the metal contact in the present case. The Fermi level of the interface is 2.2 eV above the valence-band maximum, which is by definition the barrier height ϕ_b for *p-type* diamond. This is in agreement with experimental values 1.9–2.2 eV for the diamond-Al Schottky barrier.[14] As the calculated

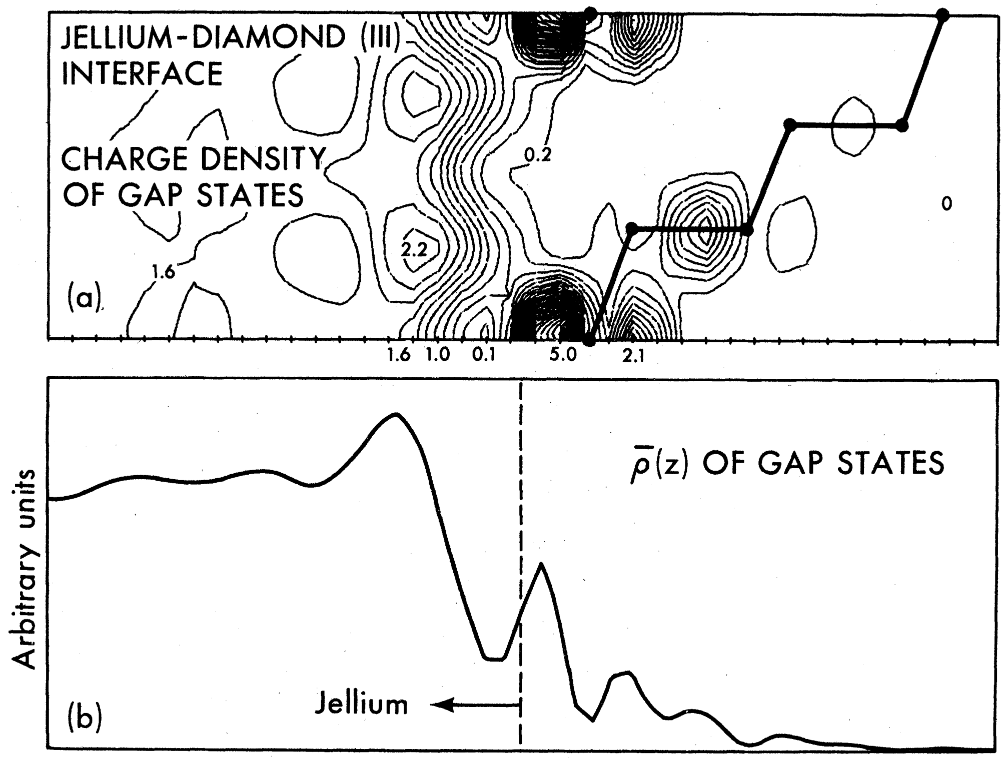

FIG. 5. (a) Charge-density contours for gap states with energies between 0 and 4 eV in a $(1\bar{1}0)$ plane. The numbers should be multiplied by 0.82 to get the number of electrons per unit cell of bulk diamond. (b) The same charge density averaged parallel to the interface and plotted along the direction perpendicular to the interface.

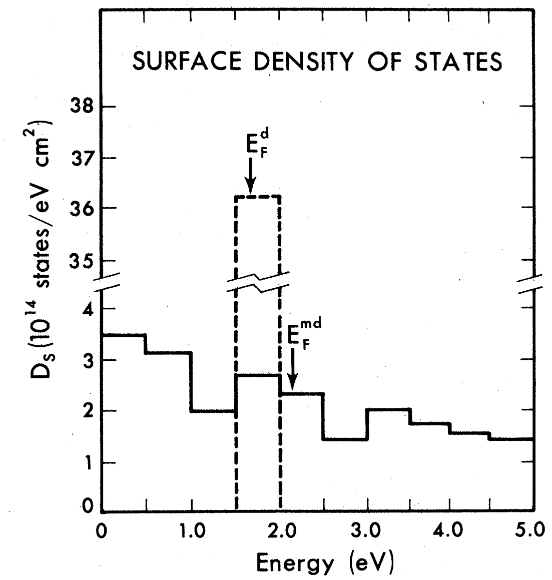

FIG. 6. Surface density of states D_s of the jellium-diamond(111) interface in the gap. Also shown (in heavy dashed lines) is the density of states of the clean diamond(111) surface states in the gap from Ref. 8. Again, the clean diamond surface-state peak is drastically reduced by the metal contact. The new metal-induced gap states give almost uniform D_s. E_F^{md} and E_F^d are defined as in Fig. 3.

indirect gap is 5.7 eV compared with the experimental value of 5.5 eV, uncertainty of ~0.2 eV is involved in determining energy levels. Spin-orbit splitting is completely negligible for diamond.

IV. THEORY OF THE SCHOTTKY BARRIERS

The results obtained in the previous section are analyzed here and the behavior of the Schottky barrier is discussed, theoretically, based on this analysis.

Empirically the barrier height ϕ_b obeys the relation

$$\phi_b(s,m) = S(s)\chi(m) + \phi_0(s)\,, \tag{5}$$

where $\chi(m)$ is the Pauling-Gordy electronegativity of the metal[15] and $S(s)$ and $\phi_0(s)$ are constants depending on the semiconductor. S is usually called the "index of interface behavior." Obviously, this is a linear approximation to the behavior of an extremely complicated many-body system. It has been reported recently[22] after extensive analysis of the available data that the slope S begins to decrease when $\chi(m)$ is large enough; i.e., S is also a function of $\chi(m)$. But S is still widely believed to be an important parameter characterizing semiconductors. Figure 7

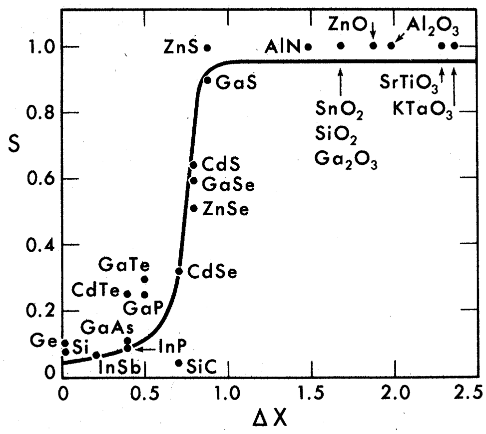

FIG. 7. Interface index S vs Pauling ionicity (from Ref. 3). For SiC the value of S has been adjusted to $S \approx 0$ (Ref. 14).

is the famous curve obtained by Kurtin *et al.*,[3] showing a rather sharp transition from covalent to ionic materials among semiconductors. Again, such a sharp transition has been questioned recently,[16] and the data are reanalyzed to show dispersed points in a bubblelike region rather than on a well-defined curve as in Fig. 7. In particular, it is found that there is nothing sacred about $S = 1.0$ saturation; S's for some materials like SiO_2 are found far above the saturated $S = 1.0$ line ($S \sim 1.5$ for SiO_2).[16] Throughout this paper S is in units of eV/(electronegativity units).

Keeping these new aspects in mind, we now use a dipole-layer model[2,17] to explain the behavior of S for different semiconductors. For a semiconductor of electron affinity χ_s in intimate contact with a metal, the electric dipole potential Δ established at the interface is

$$\Delta = \chi_s + \phi_b - \phi_m\,, \tag{6}$$

where ϕ_m is the work function of the metal. Empirically ϕ_m is found to be linear in $\chi(m)$[18]; i.e.,

$$\phi_m = A\chi(m) + B\,. \tag{7}$$

The change in Δ for a metal of slightly different $\chi(m)$ in contact with the same semiconductor is therefore

$$d\Delta = d\phi_b - A\,d\chi(m)\,. \tag{8}$$

On the other hand, since the change in Δ originated from the change in dipole charge $-eD_s(E_F)d\phi_b$, we have

$$d\Delta = -4\pi e^2 D_s(E_F)\,d\phi_b\,\delta_{\text{eff}}\,, \tag{9}$$

where δ_{eff} is the effective distance between the electrons transferred to the semiconductor side and the holes left behind in the metal. Eliminating $d\Delta$ from Eqs. (8) and (9) and using the definition, $S \equiv \partial\phi_b/\partial\chi(m)$, we get

$$S = A/[1 + 4\pi e^2 D_s(E_F)\delta_{\text{eff}}] \ . \tag{10}$$

In our derivation of Eq. (10), the formation of the M-S chemical bond is not taken into account. Chemical bonding is not believed to be crucial because we are doing a linearized Schottky-barrier theory and S has been found experimentally to be dependent only on semiconductor properties to first order. Any M-S interaction is replaced by a product of χ of the metal and S of the semiconductor in Eq. (5). The successful application of Eq. (10) to Si and zinc-blende semiconductors has been discussed previously.[2]

To calculate S from Eq. (10), we have to evaluate the effective distance δ_{eff}. This distance is the true distance divided by the appropriate dielectric screening function, i.e., $\delta_{\text{eff}} = t_m/\epsilon_m + t_s/\epsilon_s$. We may approximate t_m/ϵ_m by a typical screening length in a metal ~0.5 Å and t_s by our calculated δ in Sec. III. The dielectric constant ϵ_s for potential fluctuations over a distance of the order of δ has been found to be ~2 for both Ge (Ref. 19) and diamond.[20,21] A in Eq. (10) is taken to be 2.27 according to Gordy and Thomas.[18]

Recently, it has been pointed out that the slope A begins to decrease for large $\chi(m)$.[22] This is directly related to the dependence of S on $\chi(m)$ mentioned above and is a measure of the deviation from the linear theory. If we could leave out the contribution to the metal work function from the surface dipole of the metal, the linearity would be better. This fact was recognized by Heine in his early paper[10] and more explicitly stated in a recent paper by Schlüter,[16] but we will not go into the details of this controversal point[23] in the present paper.

Substituting our results for D_s and δ obtained in the previous section into Eq. (10), we obtain $S = 0.14 \pm 0.05$ for Ge and $S = 0.38 \pm 0.1$ for diamond. The value for Ge is in good agreement with experiment ($S\sim 0.1$). There are no acceptable experimental data for S for diamond. One experiment reported $S \sim 0.2$ or smaller for diamond,[14] but the authors pointed out that this value is not conclusive. The results are summarized in Table II. Although we calculate S without regard to the doping condition of the semiconductors, it is known experimentally that ϕ_b is practically independent of doping density for typical doping densities of $n \sim 10^{17}$ cm^{-3}.

TABLE II. Theoretical and experimental values for various parameters of the Schottky barrier. They are defined in the text.

	Ge	Diamond
D_S^{calc} (10^{14} states/eV cm^2)	4.7	2.3
δ^{calc} (Å)	2.7	1.37
ϕ_b^{expt} (eV)	~0.55 [a]	~2.0 [b]
ϕ_b^{calc} (eV)	0.55 ± 0.1	2.2 ± 0.3
S_{expt}	0.1 [c]	? (0.2) [b]
S_{calc}	0.14 ± 0.05	0.4 ± 0.1

[a] References 12 and 13.

[b] Reference 14.

[c] Reference 3.

We now present some semiquantitative interpretations of our results in terms of the energy gap E_g and the lattice constant a_c. Comparison with previous metal-Si and metal–zinc-blende semiconductor interface calculations indicates that the charge transfer per unit area to the semiconductor resulting from the exponential tail of the metal-induced states in the thermal gap is proportional to the number of surface atoms of the semiconductor per unit area. In other words, each surface atom of the semiconductor "induces" approximately a fixed amount of charge transfer from the metallic wave functions to the semiconductor side. We neglect the dependence of the density of surface atoms on the crystal face of interest [e.g., the (110) surface is a little more dense in atoms than the (111) surface] and normalize it to the density on the (111) surface. This is justified because the barrier behavior has been known[10] to be insensitive to the crystallographic orientation of the surface. We estimate that 0.6–0.7 electronic states per surface atom are available on the semiconductor side in the *thermal* gap for any of the following: Si, GaAs, ZnSe, ZnS, Ge, or diamond. If we assume that the surface density of states D_s is more or less uniformly distributed in the thermal gap, then a large gap material has a small D_s for a given number of electronic states available. Neglecting lattice constant effects, the D_s of diamond compared, say, to Si would be reduced by a factor of the ratio of their gaps, $\sim\frac{1}{5}$. (Here we used the thermal gap rather than Phillips' average gap.[24] The use of the Phillips' gap is not consistent with our argument for two reasons. First, we are interested in the two-dimensional band structure. Second, the assumption of nearly uniform D_s holds only in a narrow region of the fundmental gap; it is obviously not true for the wide energy region of the Phillips' gap. The average gap of the *two-dimensional projected band structure* would be appealing theoretically; this gap is still too wide for the uniform D_s approximation. Moreover, we have to calculate it separately while the thermal gap is an easily measurable quantity.) However, since diamond has a smaller lattice constant than Si, it has a larger number of surface atoms per unit area, hence, D_s of diamond increases by a factor of the ratio of square of the lattice constants ~2.3. The net resultant D_s for diamond would be about one half of Si, and indeed we get $\sim 2.3\times 10^{14}$ states/eV cm^2 compared with $\sim 4.5\times 10^{14}$ states/eV cm^2 for Si.[2]

δ is essentially a property of the semiconductor and determined mainly by the gap size. The decay length of the metal induced states of Ge (~2.7 Å) compares well with the decay length of the dangling-bond states of the clean Ge surface (~2.5 Å). Corresponding values for diamond are ~1.37 Å and ~1.0 Å, respectively. For completeness, we give the corresponding values for Si; they are ~3.0 and ~2.5 Å, respectively. When a M-S contact is made, δ increases by a small but finite amount in each case. At the center of the gap, δ for metal-induced states is very close to δ for dangling-bond states. As we approach the edge of the gap δ increases. So the average δ for metal-induced states is longer than the δ for dangling-bond states. This also accounts for the fact that the fractional lengthening of δ (from dangling-bond states to MIGS) is in the order of Ge, Si, diamond; i.e., in the order of increasing gap size. We may well take the value of δ for dangling-bond states if these states exist on the clean surface and if a M-S calculation is not available. A more elementary estimate of δ using the WKB approximation ($\hbar/2\delta = (m\bar{E}_g)^{1/2}$, where $\bar{E}_g$ is Phillips' average gap[24]) is also in agreement with our detailed calculation. Here, the average gap of the two-dimensional projected band structure is definitely the most appropriate one. But we can simply take Phillips' E_g. In general, S is less sensitive to δ than to D_s. It is crucial in the above arguments that D_s is approximately constant in the thermal gap. This was assumed by some of the earlier workers[17] and proved to be approximately the case in a model calculation for the Si-metal interface by Yndurain *et al.*[25] Our complete calculations show that it is always permissible to replace $D_s(E_F)$ by $\langle D_s(E)\rangle$, the average of $D_s(E)$ in the thermal gap, to calculate S.

Using the above arguments, we now examine the case of cubic SiC. SiC is also an interesting test case because S for SiC would be greater than S for Si or diamond if ionicity should be used as the characteristic parameter. From experimental data[14] the S parameter for SiC is probably very close to that of Si, although precise determination is difficult. Using Si as a reference material, and from the experimental values $E_g = 2.3$ eV and $a_c = 4.35$ Å for cubic SiC,[26] we estimate D_s for SiC compared to D_s for Si,

$$\frac{D_s^{\rm SiC}}{D_s^{\rm Si}} \sim \frac{1.1}{2.3}\left(\frac{5.43}{4.35}\right)^2 \sim 0.75\,. \tag{11}$$

Assuming the same reduction in δ we get $S\sim 0.2$ for SiC, which is half the calculated S for diamond and close to the calculated value $S = 0.13$ or the experimental value $S\sim 0.1$ for Si. Our calculation predicts $S^{\rm Si} < S^{\rm SiC} < S^{\rm diamond}$, while any model based on ionicity as the fundamental parameter would predict $S^{\rm Si} = S^{\rm diamond} < S^{\rm SiC}$.

V. CONCLUSIONS

In summary, we obtain $\phi_b = 0.55$ eV and $S = 0.14$ for Ge and $\phi_b = 2.2$ eV and $S = 0.4$ for diamond Schottky barriers. These values are in agreement with experiment where experimental data are available. $S = 0.4$ for diamond does not fit into the curve in Fig. 7 ($\Delta X = 0$ for diamond). Our result is also in contrast to recent attempts to parametrize the barrier behavior by the chemical reactivity[11] or by atomic term values,[5] which would give $S\sim 0$. If our calculation is confirmed by experiment, this would support the conclusion that the behavior of the Schottky barrier S is not primarily determined by ionicity, and a sharp transition between covalent and ionic materials can not be an appropriate description of the $S(\Delta X)$ curve. We argue in Sec. IV that $D_s \propto (E_g a_c^2)^{-1}$ using metal-induced gap states, and we are able to explain the behavior of the Schottky barrier without invoking many-body effects or chemical bond effects.

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