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Ionicity and the theory of Schottky barriers*

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We have investigated the role of ionicity in metal-semiconductor Schottky barriers by examining interfaces of increasing semiconductor ionicity. The electronic structure of four separate interfaces consisting of jellium (of Al density) in contact with the (111) surface of Si and the (110) surfaces of GaAs, ZnSe, and ZnS is investigated through the use of a self-consistent pseudopotential method. The barrier height and the surface density of states in the semiconductor band gap are determined. The phenomenological index of interface behavior S (studied by Kurtin, McGill, and Mead for semiconductors of different ionicity) is discussed in terms of a simple model involving metal-induced states in the semiconductor gap.

I. INTRODUCTION

Experimentally the behavior of the Schottky-barrier height ϕ_b for metal-semiconductor (M-s) interfaces as a function of the metal electronegativity is found to be dramatically different depending on whether the semiconductor is covalent or ionic.[1] For covalent semiconductors ϕ_b is approximately constant for all metals, whereas for ionic semiconductors, ϕ_b is strongly dependent on the metal contact. Furthermore, the transition from covalent behavior to ionic behavior appears to be a rather sharp transition which occurs at a critical ionicity.

While there have been a number of theories and speculations[2-7] and various mechanisms have been proposed to explain these properties of the barriers, a definitive explanation has yet to emerge because of the lack of detailed information on the microscopic nature of M-s interfaces. A necessary step toward understanding the properties of Schottky barriers should therefore involve a systematic study of the electronic structure of a series of M-s interfaces as a function of increasing semiconductor ionicity. Our present work is motivated by these considerations.

The electronic structure of a metal-Si interface has been studied recently[7] by two of the authors (S.G.L. and M.L.C.) using a self-consistent pseudopotential method. To circumvent the complex geometric problem of matching two crystal lattices, the metal was replaced by a jellium model in Ref. 7. Energy bands, charge densities, and the local density of states of the interface were calculated and analyzed within the one-electron theory. A barrier height in very good agreement with experiment was obtained. In this paper, we extend the analysis in Ref. 7 to the metal–zinc-blende semiconductor interfaces and present theoretical results on the microscopic origin of the ionicity-dependent behavior of M-s Schottky barriers.

The interfaces studied are interfaces of Al (modeled by a jellium core potential with $r_s = 2.07$) in contact with the ideal (111) surface of Si and the ideal (110) surfaces of GaAs, ZnSe, and ZnS. We find that, within the jellium-semiconductor model, the electronic structure of the four interfaces under investigation is qualitatively similar. Moreover we find that the experimentally observed variation in ϕ_b for different metals in contact with semiconductors of different ionicity can be understood quantitatively in terms of a simple model involving metal-induced states in the semiconductor band gap.

The remainder of the paper is organized as follows: In Sec. II the methods of calculation are discussed briefly. In Sec. III the results for the electronic structure of the metal–zinc-blende semiconductor interfaces are presented. In Sec. IV the ionicity-dependent behavior of the Schottky-barrier height is examined. And in Sec. V some discussion and conclusions are presented.

II. CALCULATIONS

As in Ref. 7 we are considering intimate M-s interfaces; i.e., there is no oxide layer between the metal and the semiconductor. We further approximate the system by replacing the metal with a jellium model and describing the semiconductor 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 at length in Ref. 7. Hence, in this section, we shall only briefly describe some of the essential features of the method and will be mainly concerned with the parameters needed in the calculations.

The 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) per-

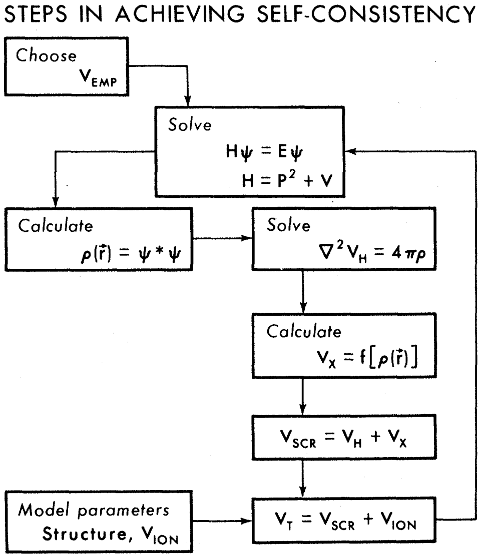

FIG. 1. Self-consistent loop in calculating the electronic structure of a metal-semiconductor interface (after Ref. 7).

iodicity is artificially retained along the direction perpendicular to the interface to allow for the use of the usual pseudopotential techniques.[8]

The calculations were carried out by constructing an elongated unit cell which, in two dimensions, is spanned by the shortest lattice vectors parallel to the appropriate semiconductor surface and, in the third dimension, by a long c axis extending over m atomic layers of the semiconductor and n layers of equivalent thickness of jellium metal. (Here the thickness of one layer is the interatomic distance between planes of semiconductor atoms parallel to the interface; and, the length of the c axis is therefore equal to $m+n$ interplane distances.) The numbers used were $m=11$ and $n=7$ for metal-GaAs and metal-ZnSe and $m=11$ and $n=9$ for metal-ZnS.

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. Since we use a jellium-semiconductor model, the structure is determined by the crystal structure of the semiconductors except for the placement of the edge of the positive jellium core. This edge has been taken to be at a distance of one-half of an interlayer distance away from the outermost semiconductor atoms. The ion core potentials used are local pseudopotentials whose Fourier transforms are of the form

$$V_{\rm ion}(q) = (a_1/q^2)[\cos(a_2 q) + a_3 q]\exp(a_4 q^4)\,, \tag{1}$$

where the parameters a_i are fit to a Heine-Abarenkov core potential.[9]

TABLE I. Ionic core potential parameters a_i. The potentials are normalized to an atomic volume of 152.3 a.u.[3] The form of the potential is given by Eq. (1). The units for $v(q)$ are Ry if q is given in a.u. (The Ga potential is valid only for $q \le 3$ a.u.)

	Ga	As	Zn	Se	S
a_1	−0.3384	−0.7057	−0.3056	−2.3258	−5.4101
a_2	1.3305	1.0448	1.3412	0.5283	0.3275
a_3	0.4466	0.1662	0.0802	−0.5740	−0.8169
a_4	0.0071	−0.0151	−0.0086	−0.0321	−0.0250

Figure 1 summarizes the self-consistent procedure employed. Screening is achieved using a Hartree potential via Poisson's equation and a Slater statistical exchange. The details of the method are given in Ref. 7. In addition to the ionic core potentials, a starting potential is needed to initiate the self-consistent loop. For this purpose we have used the empirical pseudopotentials obtained from bulk calculations with Fourier transforms expressed in a four-parameter curve of the form

$$V_{\rm emp}(q) = b_1(q^2 - b_2)/\{\exp[b_3(q^2 - b_4)] + 1\}\,. \tag{2}$$

The parameters a_i and b_i for the various semiconductors used in the calculations are listed in Tables I and II, respectively.

Using the same convergence criteria as in Ref. 7, a basis set of approximately 500 plane waves was employed in expanding the wave functions in the calculations. An additional ~1200 plane waves were also included via Lowdin's perturbation scheme.[8] The total valence charge density $\rho(\vec{r})$ needed for each iteration was determined by a five-point sampling over the irreducible part of the rectangular zone. The points included the symmetry points Γ, X, X', and M and one general point in the center of the irreducible zone.[10] This set of points yields an accurate charge density and, at the same time, allows the use of symmetrized plane waves to reduce the sizes of the Hamiltonian matrices and hence the computation time

TABLE II. Empirical starting potential parameters b_i. Normalization and units are as in Table I. The form of the potential is given by Eq. (2).

	Ga	As	Zn	Se	S
b_1	1.2214	0.3474	6.7008	0.2334	0.2361
b_2	2.4495	2.6203	1.4983	3.3858	3.3630
b_3	0.5445	0.9335	0.6696	0.7266	0.7243
b_4	−2.7148	1.5677	−4.7128	2.2012	2.1900

for diagonalization.

Upon the completion of the self-consistent loop, the various states near the interface are analyzed in terms of a local density of states (LDOS) and individual charge densities. The LDOS displays the density of states in real space near the interface and, for a given region in real space, it is given by

$$N_i(E)=\sum_{\vec{k}_{\parallel},n}\int_{\Omega_i}|\psi_{\vec{k}_{\parallel},n}(\vec{r})|^2\,d^3r\,\delta(E-E_n(\vec{k}_{\parallel}))\,, \qquad (3)$$

where $\vec{k}_{\parallel}$ is the wave vector parallel to the interface, n is the band index, ψ is the electronic wavefunction, and Ω_i is the volume of the chosen region. The physical significance of $N_i(E)$ is that it gives the probability that an electron with energy E will be found in region i.

III. ELECTRONIC STRUCTURE

In this section, the electronic structure of the three metal–zinc-blende semiconductor interfaces is presented. Some of the results have been briefly reported previously.[11]

We have chosen the interfaces M-Si, M-GaAs, M-ZnSe, and M-ZnS to study because the semiconductors composing this series are of the same crystal structure and of increasing ionicity. Within our model, we find that the calculated electronic structure of the four M-s interfaces is qualitatively very similar. In all four cases, as found in Ref. 7, the intrinsic surface states which existed in the fundamental gaps of these semiconductors[9] are removed by the presence of the metal and new types of states occur in this energy range. These metal-induced gap states[7] (MIGS) are bulklike in the metal and decay rapidly into the semiconductor with some of the characteristics of the semiconductor-vacuum surface states (which exist in the absence of the metal) weakly retained at the semiconductor surface. In addition, truly localized interface states which have charge densities decaying in both directions away from the interface are found for energies near the lower part of the semiconductor valence band.

Before we discuss the individual states, let us examine the self-consistent, valence charge densities for the three metal–zinc-blende semiconductor interfaces. They are shown in Figs. 2 to 4. In each figure the total valence charge density is displayed in two different planes containing the two types of semiconductor surface atoms. The units are normalized to one electron per unit cell. Several interesting features are seen from

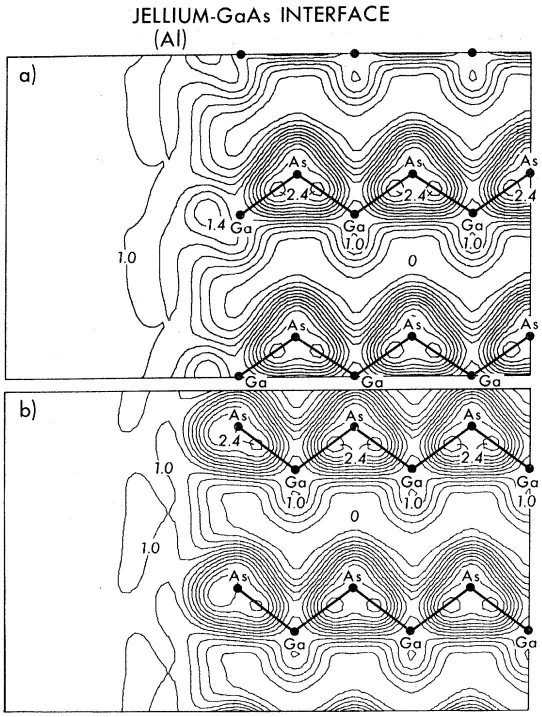

FIG. 2. Total valence charge density for the M-GaAs interface plotted in the $(1\bar{1}0)$ plane containing the (a) Ga surface atom and (b) As surface atom. The charge density has been normalized to one electron per unit cell.

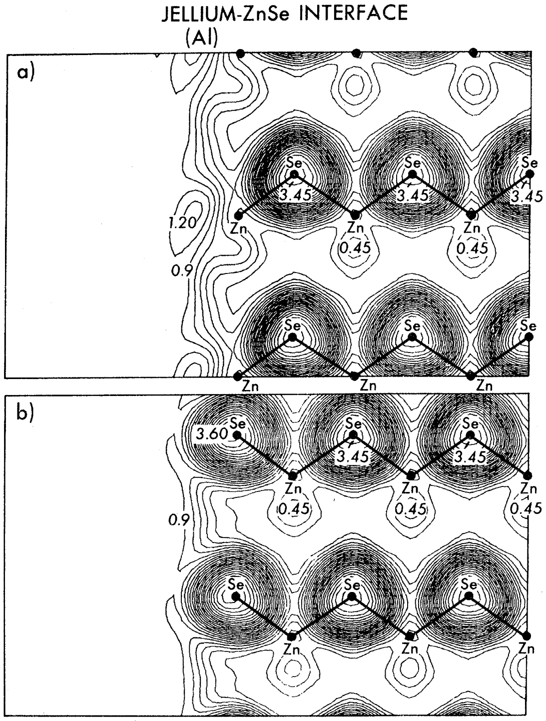

FIG. 3. Total valence charge density for the M-ZnSe interface plotted in the $(1\bar{1}0)$ plane containing the (a) Zn surface atom and (b) Se surface atom. Normalization is as in Fig. 2.

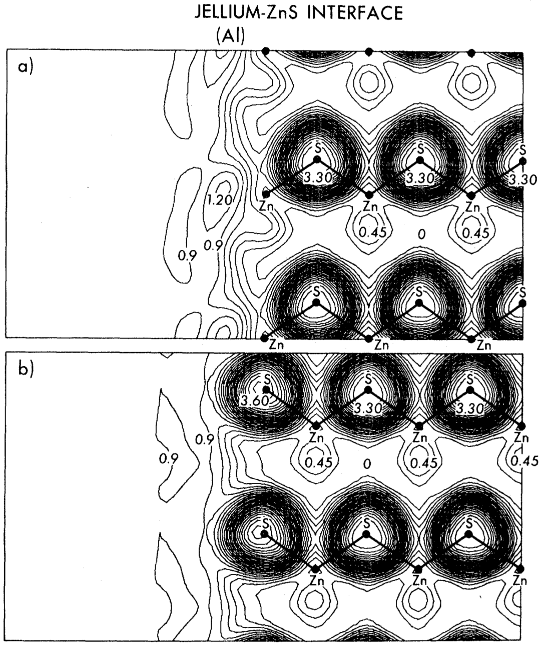

FIG. 4. Total valence charge density for the M-ZnS interface plotted in the (1$\bar{1}$0) plane containing the (a) Zn surface atom and (b) S surface atom. Normalization is as in Fig. 2.

the figures: (i) Charge densities in the bulk configuration are essentially the same as those found in the third layer into the semiconductor showing that the significant influence of the interface is quite short range (i.e. in the order of two to three atom layers); (ii) owing to the stronger potential of the anions, charge is increasingly localized on the anions as the ionicity of the semiconductor increases; and (iii) for all three interfaces, the charges on the outermost semiconductor atoms are slightly higher than the charges on the atoms deeper in the slab. This probably results from the presence of the metal which lowers the potential of the surface atoms.

In Fig. 5 the local density of states for the M-GaAs system is displayed for four regions. Each region contains one atomic layer. Region D is at the center of the semiconductor slab. Region C is the layer containing the outermost semiconductor atoms. Region B is adjacent to region C on the metallic side. The boundary between region C and B defines the interface. And finally region A is at the center of the metallic slab. The LDOS was evaluated according to Eq. (3) with five $\vec{k}$ points in the irreducible zone to calculate the histograms.[12] The LDOS for the M-ZnSe and M-ZnS interfaces are calculated in the same manner; these are shown in Figs. 6 and 7, respectively. Although the number of $\vec{k}$ points used is too

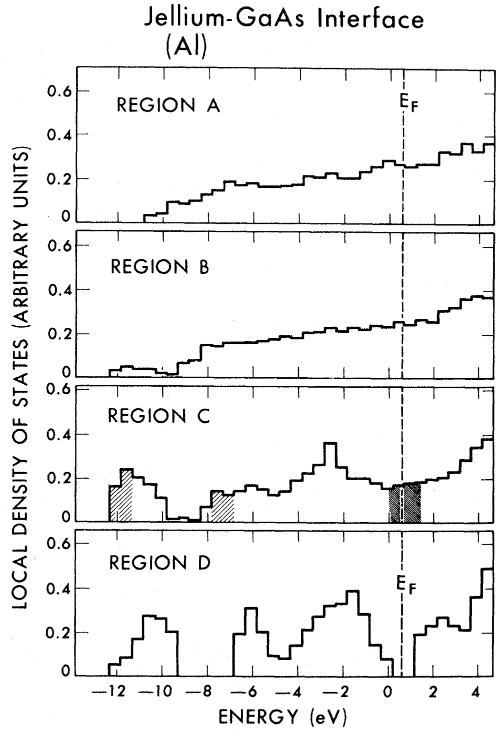

FIG. 5. Local density of states for the M-GaAs interface in arbitrary units as defined by Eq. (3).

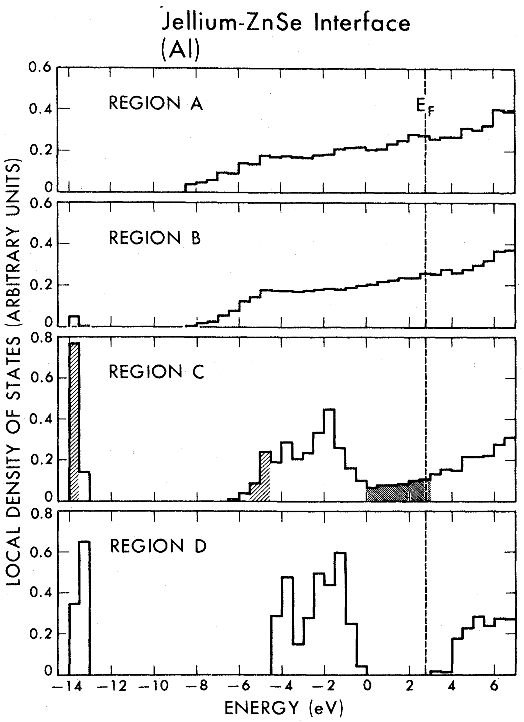

FIG. 6. Local density of states for the M-ZnSe interface.

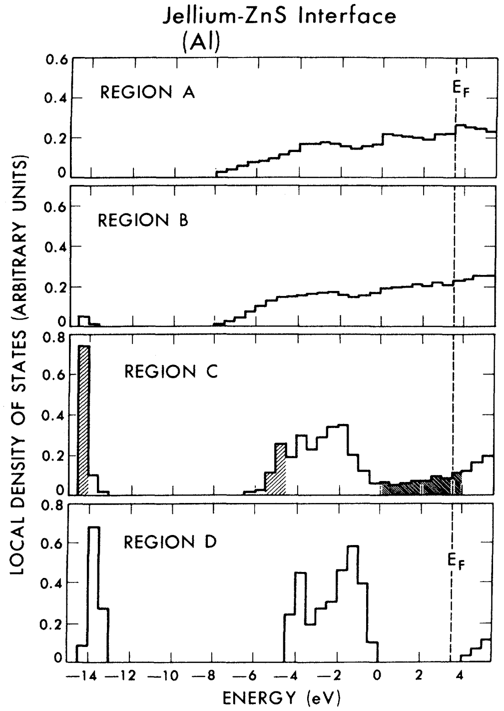

FIG. 7. Local density of states for the M-ZnS interface.

small to reproduce a nice $\sqrt{E}$ curve for the free-electron-gas density of states on the metallic side, it yields most of the prominent features of interest. A LDOS curve of much finer quality for the M-Si interface was obtained in Ref. 7 with the use of 21 $\vec{k}$ points in the irreducible zone.

The region of most physical interest is region C whose LDOS essentially describes the energy spectrum of the electrons on the semiconductor surface. The darkly shaded areas in Figs. 5–7 indicate the MIGS in the semiconductor thermal gaps. Also indicated (by the lighter shaded areas) are the energies of the localized interface states. The MIGS in the thermal gaps have, as we shall show in Sec. IV, a large influence on the Fermi level E_F and thus play a dominant role in determining the behavior of the M-s Schottky barriers.

Figure 8 displays the charge profiles $\bar{\rho}(z)/\bar{\rho}(0)$ of the penetrating tails of the MIGS in the thermal gap for the four M-s interfaces studied as a function of distance z into the semiconductor. Here $\bar{\rho}(z)$ is the charge density for the MIGS averaged over the states in the thermal gap and averaged parallel to the interface with $z=0$ at the interface. We note that the overall behavior of the charge profiles for Si and GaAs is quite similar and that the average penetration distances are considerably shorter than previously believed. The differences in the short range oscillations in the charge profiles mostly arise from the difference in the atomic arrangement between the two types of semiconductor surfaces [Si(111) and GaAs (110)].

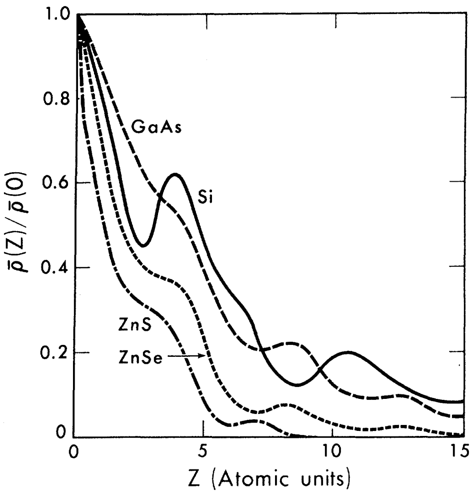

FIG. 8. Charge distributions of the penetrating tails of the MIGS in the semiconductor thermal gap. $\bar{\rho}(z)$ is the total charge density for these states averaged parallel to the interface with $z=0$ at the edge of the jellium core.

We shall only discuss and illustrate the interface states at the M-ZnS interface to avoid redundancy. The characteristics of the interface states for the other two systems are qualitatively similar. The lowest lying interface states at the M-ZnS interface (see Fig. 7) are localized strongly on the outermost sulfur atoms and have s-like character in their charge distribution. These states split off from the bottom valence band of ZnS and form a narrow interface band extending over the whole Brillouin zone. The corresponding charge density given in Fig. 9 is extremely localized on the sulfur surface atoms with practically zero charge on the zinc atoms. A surface band,

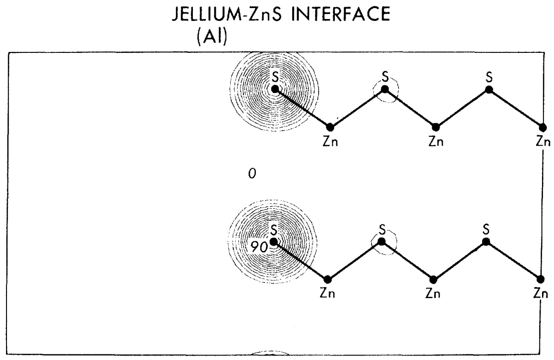

FIG. 9. Charge density of the s-like sulfur interface states in the same plane as Fig. 4(b). The charge density is again normalized to one electron per unit cell.

very similar to this s-like interface band, has been found in calculations on the (110) surface of zinc-blende semiconductors.[13] The surface states are, however, located at higher energies in the antisymmetric gap instead of at the bottom of the spectrum. These s-like interface states therefore appear to be intrinsic to the semiconductor surface with energies shifted because of the presence of the metal.

Two additional interface bands are found at ~−5 eV below the ZnS valence-band maximum. Unlike the previously discussed states, these interface states exist over a rather small region in k space at the zone edge around the point M. The charge distribution differs from the s-like state since it is p-like around the outermost sulfur atoms. The charge density for a state at M in the lower of the two interface bands is given in Fig. 10. Figure 10(a) shows the charge density contours in a $(1\bar{1}0)$ plane containing the surface Zn atoms. Figure 10(b) shows the charge density contours in a (110) plane parallel to the interface containing both types of semiconductor surface atoms. As seen from the figure, the charge is highly localized on the outermost semiconductor layer with the maxima of the p-like lobes lying in the (110) plane. The other interface state at M belonging to the higher of the two bands has a very different charge distribution which is displayed in Fig. 11. The charge is again p-like around the S atom. However, the charge lobes for this state are pointing along the backbond direction between the first layer S atoms and the second layer Zn atoms. Surface states somewhat similar to these states are also found in surface calculations.[13]

Our results are consistent with recent experiments on metal overlayers which have provided information on the electronic structure of M-s interfaces in the energy range of the semiconductor band gap. Rowe *et al.*[14] have found that the intrinsic surface states on the (111) and (100) semiconductor surfaces are removed by metallic overlayers and extrinsic metal-induced states are found within the band gap. Their findings on the Ge(110) surface is however somewhat ambiguous. Similar extrinsic metal-induced states are found but they are weaker and the intrinsic surface states appear not to be completely removed by the thin metallic overlayers.

IV. IONICITY AND SCHOTTKY BARRIERS

In this section some of the properties of M-s Schottky barriers and their relation to the calculated electronic structure are examined.

The calculated barrier heights for the four M-s interfaces studied are presented in Table III together with the measured ϕ_b.[15,16] The calculated values were obtained by determining the position of the conduction-band minimum of the bulk semiconductor relative to the Fermi level E_F via the

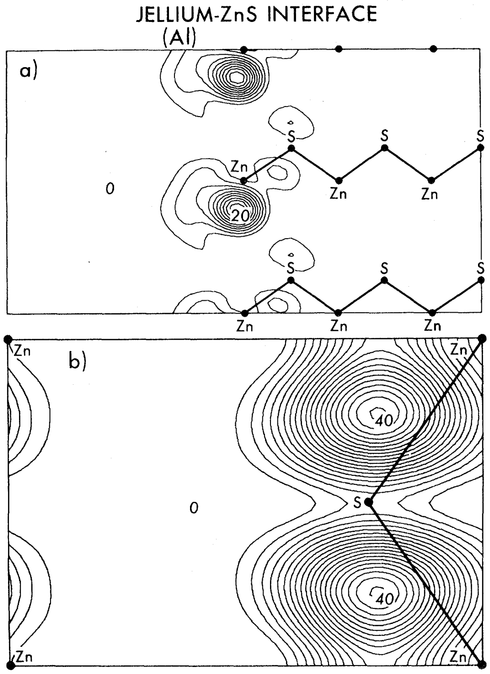

FIG. 10. Charge density of an interface state at M at −5.1 eV (see text).

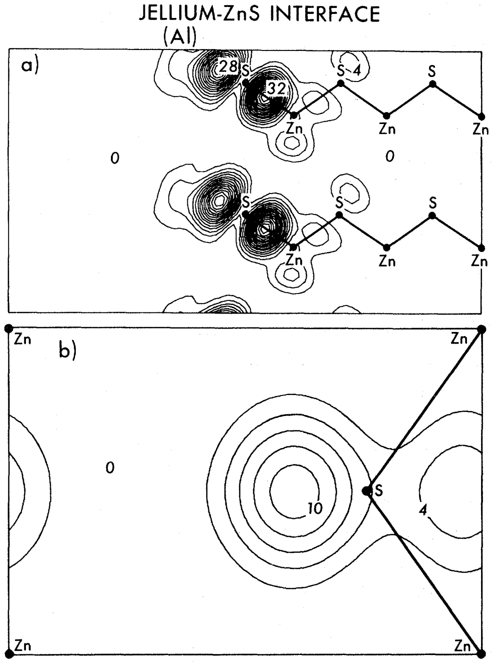

FIG. 11. Charge density of an interface state at M at −4.6 eV (see text).

TABLE III. Theoretical and experimental values for the Schottky-barrier height ϕ_b(eV) and the index of interface behavior S. D_s in units of 10^{14} states/eV cm^2 is the surface density of states used to obtain the calculated S.

	ΔX [a]	ϕ_b (cal)	ϕ_{bn} (expt)	D_s	S (cal)	S (expt) [b]
Al-Si	0	0.6 ± 0.1	0.6 [c]	4.5	0.1	0.1
Al-GaAs	0.4	0.8 ± 0.2	0.8 [d]	5.0	0.1	0.1
Al-ZnSe	0.8	0.2 ± 0.2	•••	2.0	0.4	0.5
Al-ZnS	0.9	0.5 ± 0.2	0.8 [d]	1.4	0.7	1.0

[a] Reference 17.
[b] Reference 1.
[c] Reference 16.
[d] Reference 15.

local density of states. Considering the sizes of the thermal gaps of the more ionic crystals, the agreement obtained between theory and experiment is quite good.

Empirically the barrier height $\phi_b(M,s)$ obeys the relation[1]

$$\phi_b(M,s)=S(s)X_M+\phi_0(s)\,, \tag{4}$$

where X_M is the Pauling-Gordy electronegativity[17] of the metal and S and ϕ_0 are constants depending on the semiconductor. As an example, the experimental barrier heights[15,16] for our four semiconductors are presented in Fig. 12 as a function of the X_M of various metals. Moreover the slope or "index of interface behavior" S is found to be a smooth function of $\Delta X=X_A-X_B$, the electronegativity difference of the anions and cations in the semiconductor. Since ΔX provides a measure of the ionicity of the semiconductor, S is also a function of the semiconductor ionicity. For ϕ_b expressed in units of electron volts, S is small ~0.1 for semiconductors with $\Delta X<0.5$ but S is ~1.0 for semiconductor with $\Delta X>0.9$. In addition, there is a well defined and rather sharp transition in the value of S at ΔX~0.7 to 0.8 (see Fig. 13).

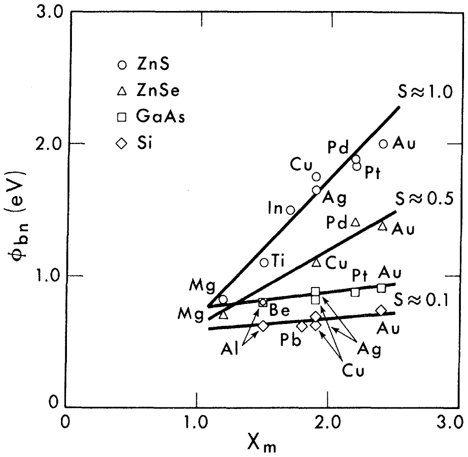

FIG. 12. Experimental values of the barrier heights for four semiconductors in contact with various metals. X_M is the electronegativity of the metal in the Pauling-Gordy scale. Data were taken from Refs. 16 (Si) and 15 (GaAs, ZnSe, ZnS).

The standard explanation for S relies on the Bardeen model which attributes this behavior of ϕ_b to the density of surface states existing in the semiconductor band gap. However arguments had been presented by Heine[3] which showed that semiconductor surface states do not exist in the fundamental gap for most M-s interfaces and many alternate theories have since been proposed.[3-7]

Physically the barrier height is determined by the requirement that in equilibrium the Fermi levels of two materials in contact are equal. This is achieved by creating an electric dipole potential Δ at the interface. Hence, in the one-electron theory, the density of the MIGS in the semiconductor thermal gap and their penetration into the semiconductor will strongly influence the behavior of ϕ_b. The extent of their penetration can be measured by a penetration depth δ defined by $\bar\rho(\delta)/\bar\rho(0)=1/e$. From Fig. 8, δ is equal to ~3.0 and ~2.8 Å for Si and GaAs, respectively. As the ionicity of the semiconductor increases, δ however rapidly reduces to ~1.9 Å for ZnSe and to ~0.9 Å for ZnS.

The other quantity which is relevant to the behavior of ϕ_b and related to the MIGS is the surface density of states $D_s(E)$. For energies in the semiconductor thermal gap, we define

$$D_s(E)=A^{-1}\int_A\int_0^\infty N(E,\vec r)\,dz\,dA\,,\quad 0\leqslant E\leqslant E_g\,, \tag{5}$$

where A is the interface area, $N(E,\vec r)$ is the LDOS as defined in Eq. (3), and the integral over z is to be evaluated from the interface to deep into the

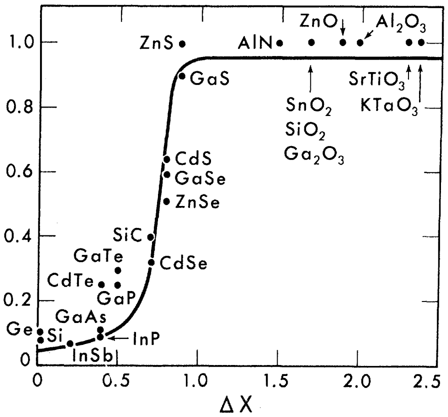

FIG. 13. Index of interface behavior S from Ref. 1.

bulk of the semiconductor. Thus $-eD_s(E)$ gives the density of localized surface charge per unit energy on the semiconductor surface. The calculated $D_s(E)$ are depicted in Fig. 14. The averaged D_s near the center of the gap for Si and GaAs which both have about the same S is approximately the same. Two trends which can be observed from Fig. 14 are that $D_s(E)$ decreases for more ionic semiconductors and $D_s(E)$ has a relatively flat minimum over the center region of the gap. The D_s for M-ZnSe is essentially identical to that of M-ZnS except its magnitude is ~30% higher. Hence it is omitted from Fig. 14.

From an electrostatic point of view, the fact that both δ and D_s decrease for more ionic semiconductor crystals implies that the change in Δ with respect to a change in E_F will be small for ionic semiconductors and larger for covalent semiconductors. Therefore we expect from the calculated δ and D_s that S will be large for ionic crystals and small for covalent crystals.

To estimate the influence of δ and D_s on the barrier height, we use the following simple model to calculate $S(s)$. Cowley and Sze[18] had used a somewhat similar approach to obtain the interface density of states in terms of the experimentally determined S. In this model, δ and D_s are assumed to be quantities intrinsic to the semiconductor (i.e., they are independent of the metal contacts) and also D_s is taken to be approximately constant over the central portion of the thermal gap. Calculations on metal-Si interfaces using surface Green's -function methods have shown that D_s is approximately constant for a wide range of metals.[5,19] In this model, we have also made use of the empirical relation that the metal work function ϕ_M is linear in X_M, i.e., $\phi_M = AX_M + B$ with $A = 2.27$ and $B = 0.34$ for ϕ_M expressed in electron volts.[17,20]

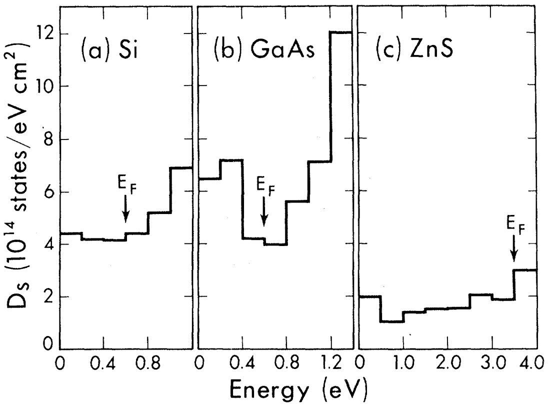

FIG. 14. Surface density of states as defined in Eq. (5).

For a semiconductor of electron affinity χ_s in contact with a metal, the electric-dipole potential established at the interface can be approximated as

$$\Delta = \chi_s + \phi_b - AX_M - B\,. \tag{6}$$

The change in Δ for a metal of slightly different X_M in contact with the same semiconductor is therefore

$$d\Delta = d\phi_b - A dX_M\,. \tag{7}$$

Using simple electrostatic arguments, another expression for $d\Delta$ is

$$d\Delta = -4\pi e^2 D_s \delta_{\mathrm{eff}} d\phi_b\,, \tag{8}$$

where δ_{eff} is the effective distance between the center of mass of the negative charge transferred to the semiconductor due to the change in ϕ_b and the center of mass of the positive charge left behind in the metal. This distance is the true distance divided by the appropriate dielectric screening function ϵ, i.e., $\delta_{\mathrm{eff}} = (t_M/\epsilon_M + t_s/\epsilon_s)$. We may approximate t_s by our calculated δ and t_M/ϵ_M by the typical screening length in a metal which is ~0.5 Å. Equations (4), (7), and (8) then yield the following S (see Ref. 21):

$$S = 2.3/[1 + 4\pi e^2 D_s(0.5 + \delta/\epsilon_s)]\,. \tag{9}$$

The dielectric screening for potential fluctuations in the distance of the order of δ has been found to be ≈ 2 by Walter and Cohen[22] for our four semiconductors. Hence we may evaluate S using the calculated values of δ and D_s and $\epsilon_s = 2$. They are presented in Table III together with the experimentally determined S. The agreement between theory and experiment is surprisingly good for this very simple model. We note here that, within our model, S is a function of *both* D_s and δ. Although our results are for intrinsic semiconductors at zero temperature, the calculated ϕ_b and S will be essentially the same as those for doped semiconductors at finite temperature. The argument is as follows, for typical doping density of $n \leq 10^{17}$ cm^{-3}, a small charge accumulation of ~10^{12} electrons/cm^2 at the semiconductor surface will result in band bending on the order of volts. Hence, with $D_s \sim 10^{14}$/eV cm^2, only a slight change (~0.01 eV) in E_F at the interface is needed to account for the band bendings caused by impurities or thermally excited electrons.

We have also examined the sensitivity of our results to the only uncertain parameter in the calculations, i.e., the placement of the jellium core edge. Our results appear to be quite insensitive to this parameter. In the case of the M-Si interface, a change of 25% in this parameter left ϕ_b and δ essentially unchanged and only changed D_s by a few percent. A similar observation has been made by Louis *et al.*[5,21] They have performed non-self-consistent calculations on *M*-*s* interfaces using a Green's-function method.

V. SUMMARY AND CONCLUSIONS

Using a self-consistent pseudopotential method, we have studied the electronic structure of a series of *M*-*s* interfaces of increasing semiconductor ionicity. Our results are consistent with recent experiments on metal overlayers which indicated that the intrinsic surface states on the semiconductor surfaces are removed by metallic overlayers and extrinsic metal-induced states are found within the energy range of the band gap. Hence, contrary to the Bardeen model and the recent speculations made by Eastman and Freeouf,[23] intrinsic semiconductor surface states do not appear to play a dominant role in determining ϕ_b. Detailed experimental information on the electronic structure of these *M*-*s* is however not available at present for comparison.

We have also examined the question of ionicity in the behavior of Schottky-barrier heights. A simple model involving the MIGS has been constructed to estimate *S*. We find that both ϕ_b and *S* can be satisfactorily determined using the self-consistent pseudopotential results for the more covalent semiconductors and somewhat less accurately for the more ionic semiconductors. Our results suggest that the important properties of Schottky barriers are mostly incorporated in the one-electron jellium-semiconductor type of model. Other effects not included in the present calculations such as many-body effects and bonding between metal and semiconductor atoms are most likely necessary before complete agreement between theory and experiments for the more ionic semiconductors can be achieved.

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