Properties of interface Shockley states for a one-dimensional sp hybrid lattice

E-Ni Foo

Department of Physics and Atmospheric Science, Drexel University, Philadelphia, Pennsylvania 19104

How Sen Wong

Institute of Physics, National Tsing Hua University, Hsinchu, Taiwan, Republic of China
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The electronic density of states at the interface of two semi-infinite linear chains consisting of atoms with sp orbitals is investigated using the Green's-function formalism. The effect of the interface coupling on the Shockley surface states and the bulklike densities of states is studied in detail.

I. INTRODUCTION

Electronic states localized at the surface of a semiconductor[1-10] or at the interface between two semiconductors[11-13] have been studied by many authors because of their importance in developing semiconductor devices like junction transistors. For most semiconductors, such as tetrahedrally coordinated Si, Ge, and GaAs, their electronic structure can be well constructed by tight-binding combinations of bonding sp hybrid orbitals.[14,15] As noted by Shockley in 1939,[1] surface states appear at the middle of the energy gap when the s and p bands cross, even if no surface potential perturbation is present. In contrast to the Tamm surface state,[2] whose existence solely depends on the potential perturbation at the surface, such a surface state is called a *Shockley surface state*. It is known that the appearance of the gap states will severely modify the optical and electrical properties of a semiconductor. Thus a study of the effect of the interface coupling between two semi-infinite semiconductors on the Shockley states is of interest.

Shockley[1] considered a general one-dimensional crystal, containing a finite number of atoms with symmetric potential wells. He used the method of matching the wave function and its derivative at the crystal surface. Goodwin[3] studied a similar problem based on the linear-combination-of-atomic-orbitals (LCAO) method. The LCAO method was later generalized by many authors to study the existence conditions and energies of the various types of surface states.[4,5]

Most recently, Foo and Wong[6] (FW) made a systematic study of the Shockley surface state for a one-dimensional tight-binding model, using the more sophisticated Green's-function method. This Green's-function method was outlined in detail by Kalkstein and Soven[7] (KS). This method is ideal for treating tight-binding crystals consisting of atoms with localized orbitals. FW were able to study the Shockley state analytically. The essence of the KS method can be summarized as follows: The surface of a semi-infinite crystal is formed by starting with a perfect (infinite) crystal and passing an imaginary cleavage plane through it in some crystallographic direction. The hopping integrals which couple the two cleaved crystals are set equal to zero. The difference between the Hamiltonians of the perfect and cleaved crystals is then treated as a scattering potential. Thus the Green's functions for the cleaved crystals can be expressed in terms of the Green's function for the perfect crystal and the scattering potential introduced by the cleavage plane.

Properties of Shockley surface states have also been investigated via the pseudopotential method[8-10] with complex band structure. In this treatment, the electrons in the crystal were regarded as nearly free, the crystal was treated as a continuum, and the potential was regarded as a perturbation. The Shockley state was found to exist inside the bonding energy gap (crossed band) but not in the antibonding energy gap (uncrossed band).

Electronic interface states have also been studied, primarily along the line of either the LCAO method or the pseudopotential method. Davison and Cheng[11] studied the interface state of a composite crystal using the LCAO method. Since the hybridization of the sp orbitals was not included in their model, a Shockley state did not appear in their calculations. Garcia-Moliner and Rubio[12] extended the pseudopotential method to study the *interface* Shockley state. However, it is again applicable to a nearly-free-electron model. Parallel to the development of the theory of the interface electronic states, studies on interface phonon state were also reported by Maradudin *et al.*[16] and Hori *et al.*[17] However, no Shockley-type state appeared in phonon spectrum.

The purpose of this paper is to use the Green's-function formalism to study the interface Shockley states. The interface is formed along the line as suggested by Maradudin *et al.*[16] A pair of cleaved semi-infinite crystals are coupled together via

an interface hopping integral. Then the pair of cleaved semi-infinite crystals are regarded as the unperturbed system and the interface hopping integral is treated as the scattering potential. Thus the interface Green's function can be expressed in terms of the surface Green's functions associated with the pair of cleaved semi-infinite crystals and the interface hopping integral.

In Sec. II, the Green's-function formalism for the interface states is derived for a tight-binding model. In Sec. III, application of this formalism to a one-dimensional sp hybrid model is presented. A brief discussion of the conclusions is given in Sec. IV.

II. GREEN'S-FUNCTION FORMALISM FOR INTERFACE STATES

In this section we will derive a formalism for the interface electronic states in general. Our derivation is similar in spirit to that outlined by Maradudin et al.[16] in their studies of the interface phonon spectrum. The interface is formed by coupling the cleavage planes of a pair of semi-infinite crystals. The atomic orbitals in both crystals are assumed to be localized at the lattice sites; i.e., they are mutually orthogonal. All hopping integrals, except those between the nearest neighbors, are assumed to be negligible. Let H_{RR} and H_{LL} be the Hamiltonians for the right-half (RH) and left-half (LH) semi-infinite cleaved crystal and H_{RL} (or H_{LR}) represent the interaction between RH and LH crystals which consists of the nearest-neighbor hopping integrals between atoms located on the two cleaved surfaces. Let H denote the interface Hamiltonian for the coupled RH and LH crystal, which can be expressed as

$$H = \begin{pmatrix} H_{RR} & H_{RL} \\ H_{LR} & H_{LL} \end{pmatrix} , \tag{1}$$

and its corresponding interface Green's function is given by

$$G = \begin{pmatrix} G_{RR} & G_{RL} \\ G_{LR} & G_{LL} \end{pmatrix} = (E - H)^{-1} . \tag{2}$$

The calculations are facilitated by the observation that the whole system retains a translational symmetry parallel to the interface plane. For convenience we will adopt a mixed Bloch-Wannier representation in the following derivations. Thus the wave functions can be specified as $|K_{\parallel}, n\rangle$, where $K_{\parallel}$ is the wave vector parallel to the interface plane; $n = 0, 1, 2$ or $n = -1, -2$ denotes planes of lattice sites in the RH or LH crystal, and the interface is located between the $n = 0$ and $n = -1$ planes.

Since $K_{\parallel}$ is a well-defined quantum number, we will calculate the Green's functions as functions

of $K_{\parallel}$. The $K_{\parallel}$ argument will be generally suppressed in our notation, i.e., $|K_{\parallel}, n\rangle \equiv |n\rangle$. Since the Green's function corresponding to a cleaved semi-infinite crystal is known, we can treat the system consisting of two uncoupled half-crystals as the unperturbed system with the Hamiltonian

$$H' = \begin{pmatrix} H_{RR} & 0 \\ 0 & H_{LL} \end{pmatrix} , \tag{3}$$

and its associated Green's function

$$G' = \begin{pmatrix} G'_{RR} & 0 \\ 0 & G'_{LL} \end{pmatrix} , \tag{4}$$

where

$$G' = (E - H')^{-1} . \tag{5}$$

The interaction H_{RL} (and H_{LR}) is then treated as the scattering potential,

$$V = \begin{pmatrix} 0 & H_{RL} \\ H_{LR} & 0 \end{pmatrix} . \tag{6}$$

Thus the interface Hamiltonian can be expressed as

$$H = H' + V . \tag{7}$$

The interface Green's function can then be expressed in terms of the unperturbed surface Green's function G' and the scattering potential V via the Dyson equation

$$G = G' + G' V G . \tag{8}$$

For simplicity, we assume that V has only matrix elements between 0 and -1, i.e., $V(0, -1)$ and $V(-1, 0)$, then Eq. (8) can be solved exactly as follows:

$$G_{RR}(m, m) = G'_{RR}(m, m) + G'_{RR}(m, 0)$$
$$\times H_{RL}(0, -1) G_{LR}(-1, m),$$
$$G_{LR}(-1, m) = G'_{LL}(-1, -1) H_{LR}(-1, 0) G_{RR}(0, m) ,$$
$$G_{RR}(0, m) = G'_{RR}(0, m) + G'_{RR}(0, 0) \tag{9}$$
$$\times H_{RL}(0, -1) G_{LR}(-1, m) .$$

From (9) we obtain

$$G_{RR}(m, m) = G'_{RR}(m, m) + G'_{RR}(m, 0) H_{RL}(0, -1)$$
$$\times \Delta_{LL}^{-1} G'_{LL}(-1, -1) H_{LR}(-1, 0) G'_{RR}(0, m) , \tag{10}$$

where

$$\Delta_{LL} = 1 - G'_{LL}(-1, -1) H_{LR}(-1, 0) G'_{RR}(0, 0) H_{RL}(0, -1) .$$

Following the same procedure, we can also obtain

$$G_{LL}(-m, -m) = G'_{LL}(-m, -m)$$
$$+ G'_{LL}(-m, -1) H_{LR}(-1, 0) \Delta_{RR}^{-1} G'_{RR}(0, 0)$$
$$\times H_{RL}(0, -1) G'_{LL}(-1, m) , \tag{11}$$

where

$$\Delta_{RR} = 1 - G'_{RR}(0,0) H_{RL}(0,-1) G'_{LL}(-1,-1)$$
$$\times H_{LR}(-1,0) .$$

The surface Green's function can be calculated using the KS formalism, namely,

$$G'_{RR}(m,n) = G^0_{RR}(m-n) - G^0_{RR}(m+1) H^0_{RR}(-1)$$
$$\times [1 + G^0_{RR}(1) H^0_{RR}(-1)]^{-1} G^0_{RR}(-n) , \quad (12)$$

and

$$G'_{LL}(-m,-n) = G^0_{LL}(n-m) - G^0_{LL}(-m) H^0_{LL}(-1)$$
$$\times [1 + G^0_{LL}(1) H^0_{LL}(-1)]^{-1} G^0_{LL}(n-1) , \quad (13)$$

where $G^0_{RR}(G^0_{LL})$ and $H^0_{RR}(H^0_{LL})$ represent the Green's function and the Hamiltonian for an infinite extended RH- (LH-) type crystal, respectively.

The local density of states (LDS) of the coupled crystals is given by the usual formula

$$\rho_R(m) = \frac{1}{\pi} \frac{1}{N_{\parallel}} \sum_{K_{\parallel}} \text{Im } G_{RR}(m,m) ,$$

$$\rho_L(-m) = \frac{1}{\pi} \frac{1}{N_{\parallel}} \sum_{K_{\parallel}} \text{Im } G_{LL}(-m,-m) , \quad (14)$$

where $N_{\parallel}$ is the total number of atoms in each plane

The energies of interface states are determined by the zeros of the determinant

$$\Delta \equiv \left| 1 - G'_{RR}(0,0) H_{RL}(0,-1) \right.$$
$$\left. \times G'_{LL}(-1,-1) H_{LR}(-1,0) \right| = 0 . \quad (15)$$

III. APPLICATIONS: SHOCKLEY INTERFACE STATES IN A ONE-DIMENSIONAL sp HYBRID LATTICE

Let us consider two semi-infinite one-dimensional monatomic chains, which are coupled to-gether at the interface (i. e., a point). Associated with each atom is one s-like and one p-like orbital. The interface is chosen to be between the -1 and 0 sites. The Hamiltonian for the RH crystal is given by[6]

$$H'_{RR} = \begin{pmatrix} H_{Rss} & H_{Rsp} \\ H_{Rps} & H_{Rpp} \end{pmatrix} , \quad (16)$$

where

$$H_{Rss} = \epsilon_{Rs} \sum_{n=0}^{\infty} |n,s\rangle \langle n,s|$$
$$- h_{Rss} \sum_{n=0}^{\infty} (|n+1,s\rangle \langle n,s| + |n,s\rangle \langle n+1,p|) ,$$

$$H_{Rpp} = \epsilon_{Rp} \sum_{n=0}^{\infty} |n,p\rangle \langle n,p|$$
$$+ h_{Rpp} \sum_{n=0}^{\infty} (|n+1,p\rangle \langle n,p| + |n,p\rangle \langle n+1,p|) ,$$

$$\quad (17)$$

$$H_{Rsp} = H_{Rps} = h_{Rsp} \sum_{n=0}^{\infty} (|n,s\rangle \langle n+1,p| - |n+1,s\rangle \langle n,p|) .$$

Here ϵ_{Rs} and ϵ_{Rp} represent the atomic energies of the s and p orbitals for an isolated atom, respectively. The parameters h_{Rss}, h_{Rpp}, and h_{Rsp}, respectively, represent the hopping integrals between two s orbitals, two p orbitals, and one s and one p orbital associated with two nearest-neighboring atoms. The Hamiltonian H_{LL} for the LH crystal has the same form as H_{RR} except parameters are replaced by ϵ_{Ls}, ϵ_{Lp}, h_{Lss}, h_{Lpp}, and h_{Lsp} and n is summed from -1 to $-\infty$. For simplicity, and without sacrificing too much physical content, we set $h_{Rss} = h_{Rpp} = h_{Rsp} = h_R$ and $h_{Lss} = h_{Lpp} = h_{Lsp} = h_L$. The analytical expression for G^0_{RR}(or G^0_{LL}) for this infinite one-dimensional s-p hybrid model has been calculated by Foo and Wong,[6] as

$$G^0_{ss}(n) = (1/2\epsilon) \{\delta_{n0} + [(\epsilon-E)/2\epsilon - \beta][-\beta + (\beta^2-1)^{1/2}]^{|n|} (\beta^2-1)^{-1/2}\} ,$$

$$G^0_{pp}(n) = (-1/2\epsilon) \{\delta_{n0} + [(\epsilon+E)/2\epsilon - \beta][-\beta + (\beta^2-1)^{1/2}]^{|n|} (\beta^2-1)^{-1/2}\} , \quad (18)$$

$$G_{ps}(n) = -G_{sp}(n) = (1/2\epsilon) \text{sgn}(n)(1-\delta_{n0})[-\beta + (\beta^2-1)^{1/2}]^{|n|} ,$$

where $\beta = (\epsilon^2 + 4h^2 - E^2)/4\epsilon h$ and E is measured from the middle of the energy gap, i.e., by setting $\epsilon_{Rs} + \epsilon_{Rp} = 0$ (or $\epsilon_{Ls} + \epsilon_{Lp} = 0$). ϵ is equal to $\epsilon_R \equiv \frac{1}{2}(\epsilon_{Rp} - \epsilon_{Rs})$ or $\epsilon_L \equiv \frac{1}{2}(\epsilon_{Lp} - \epsilon_{Ls})$, and h is equal to h_R or h_L. It has also been shown that a Shockley surface state appears at $E = 0$, when $\gamma_R(\equiv 2h_R/\epsilon_R)$ or γ_L $(\equiv 2h_L/\epsilon_L)$ is greater than 1, i.e., the s and p bands cross each other. Thus these s-p hybrid solids

can be classified as crossed-band or uncrossed-band types of solid.

The scattering potential at the interface is also assumed to be characterized by a single parameter h_{RL}, which reads

$$H_{RL}(0,-1) = \begin{pmatrix} -h_{RL} & -h_{RL} \\ h_{RL} & h_{RL} \end{pmatrix}$$

and

$$H_{LR}(-1,0)= \begin{pmatrix} -h_{RL} & h_{RL} \\ -h_{RL} & h_{RL} \end{pmatrix} \quad . \tag{19}$$

Thus we will consider the interface which can be characterized by the set of parameters ϵ_R, ϵ_L, h_R, h_L, and h_{RL}. In the following we will compute the electronic density of states at various kinds of interfaces, using Eqs. (11)–(14), (18), and (19).

Interaction between two degenerate Shockley states. First we consider the case in which both RH and LH crystals are band crossed, i.e., $\gamma_R > 1$ and $\gamma_L > 1$ and their Shockley states are degenerate at $E = 0$. In the presence of a weak interface coupling h_{RL}, the pair of degenerate Shockley states associated with the RH and LH crystal interact, and their energies are shifted by the amount

$$E_I = \pm 2h_{RL}[(1 - \gamma_R^{-2})(1 - \gamma_L^{-2})]^{1/2} \quad . \tag{20}$$

For the special case in which RH and LH crystals are of the same type, Eq. (20) becomes

$$E_I = \pm 2h_{RL}(1 - \epsilon^2/4h^2) \quad . \tag{21}$$

This type of interface describes the case of a weakening bond in an otherwise perfect one-dimensional lattice. However, this statement may not be applicable to a two- or three-dimensional system. In Fig. 1 the energies of interface states E_I
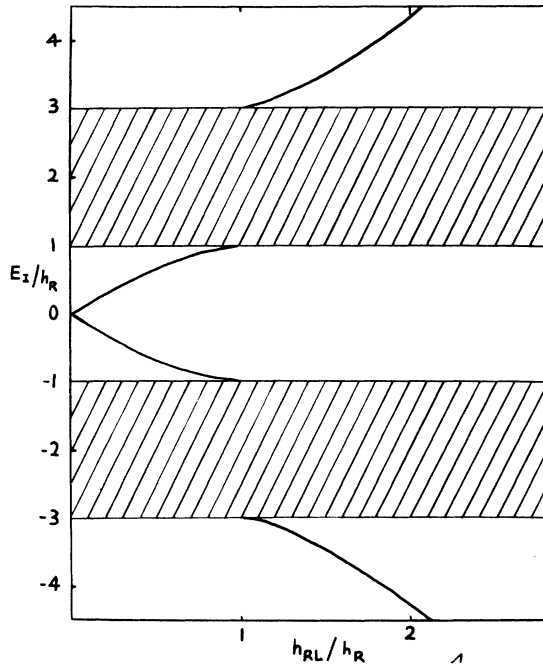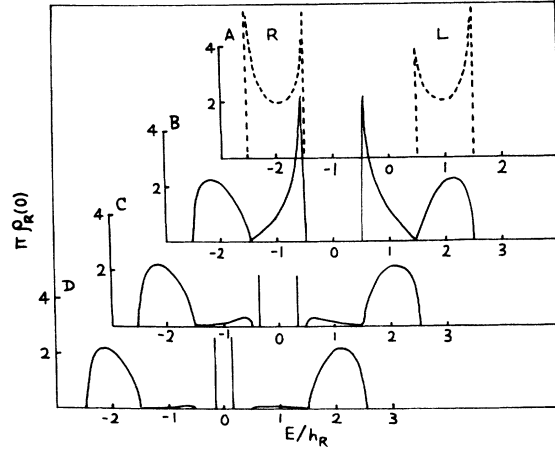

FIG. 2. Local densities of states $\rho_R(0)$ at the interface for several different h_{RL} plotted as functions of E. In (a) the dash lines represent the upper-half and the lower-half of the spectra for $\mathrm{Im}G_L^0(0)$ and $\mathrm{Im}G_R^0(0)$, respectively. (b), (c), and (d) describe $\rho_R(0)$ for $h_{RL}/h_R = 0.4$, 0.2, and 0.1, respectively. Other parameters are $\epsilon_R/h_R = \epsilon_L/h_R = h_L/h_R = 0.5$. The Shockley states are degenerate at $E = 0$ when $h_{RL} = 0$.

for this special case, with $\epsilon_R/h_R = \epsilon_L/h_R = h_L/h_R = 1$, are plotted as a function of h_{RL}. One observes that, for $h_{RL} \ll h_R$, E_I are linear in h_{RL}, as described by Eq. (21), and approach the limits of
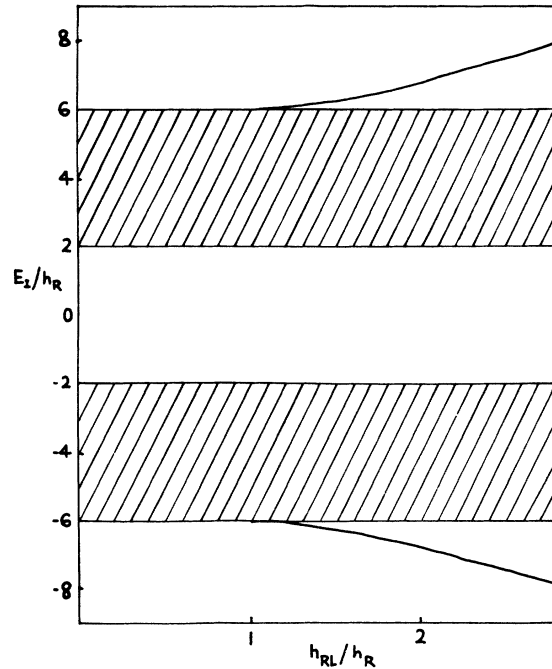

FIG. 1. Energies of the interface states E_I plotted as functions of the interface coupling constant h_{RL}. Parameters are $\epsilon_R/h_R = \epsilon_L/h_R = h_L/h_R = 1$. For such a system, both RH and LH crystals are band crossed and their Shockley states are degenerate at $E = 0$ when $h_{RL} = 0$. Shaded areas denote the bulk continuum.

FIG. 3. Energies of the interface states E_I plotted as functions of the interface coupling constant h_{RL}. Parameters are $\epsilon_R/h_R = \epsilon_L/h_R = 4$, and $h_L/h_R = 1$. For this system, both RH and LH crystals are band uncrossed.
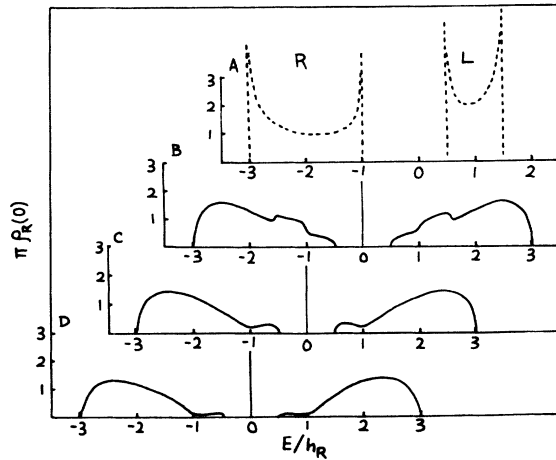
FIG. 4. Local densities of states $\rho_R(0)$ at the interface for several different h_{RL} plotted as functions of E. The parameters for this system are $\epsilon_R/h_R = \epsilon_L/h_R = 1$, and $h_L/h_R = 0.25$. For such a system, the RH crystal is band crossed and LH crystal is band uncrossed. In (a), the dash lines represent the upper- and lower-halves of the spectra for $\mathrm{Im}G_L^0(0)$ and $\mathrm{Im}G_R^0(0)$, respectively. (b), (c), and (d) describe $\rho_R(0)$ for $h_{RL}/h_R = 0.4$, 0.2, and 0.1, respectively.

$$E_I = \pm 2h_{RL}(h_R/\epsilon_R) \,, \qquad (22)$$

when $h_{RL} \gg h_R$. In Fig. 2, we consider the electronic density of state for a more general degenerate case in which the RH and LH crystals are not alike. The set of parameters is $\epsilon_L/h_R = \epsilon_R/h_R = h_L/h_R = 0.5$. For the purpose of comparison, $\mathrm{Im}G_{RR}^0(0)$ and $\mathrm{Im}G_{LL}^0(0)$ corresponding to perfect crystals are plotted in Fig. 2(a) (only one-half of the spectra being plotted here). For $h_{RL}/h_R = 0.1$,
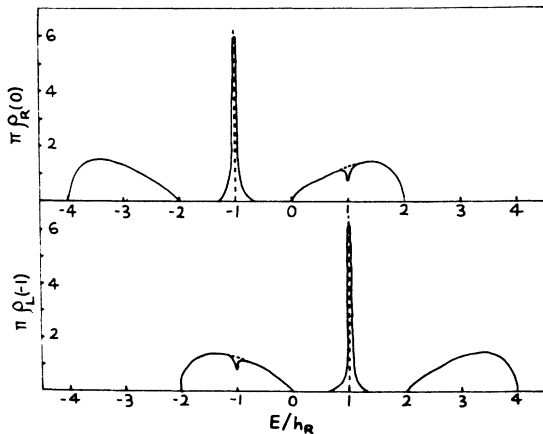

FIG. 5. Local densities of states $\rho_R(0)$ and $\rho_L(-1)$ plotted as functions of E. Parameters for this system are $\epsilon_R/h_R = \epsilon_L/h_R = h_L/h_R = 1$ and $h_{RL}/h_R = 0.1$. The centers of the energy gap for the RH and LH crystals are at $E/h_R = -1$ and 1, respectively.
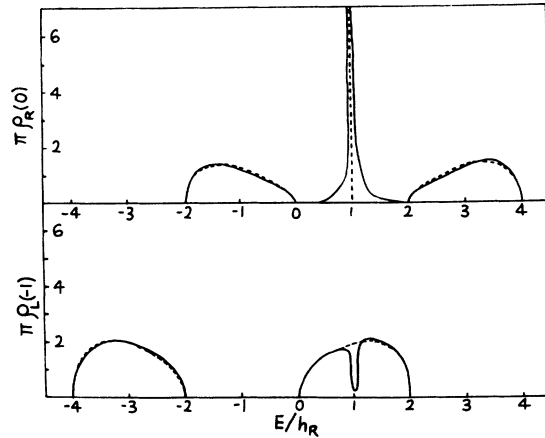

FIG. 6. Local densities of states $\rho_R(0)$ and $\rho_L(-1)$ plotted as functions of E. Parameters for this system are $\epsilon_R/h_R = 1$, $\epsilon_L/h_R = 2$, $h_L/h_R = 0.5$, and $h_{RL}/h_R = 0.1$. The centers of the energy gap for the RH and LH crystals are at $\epsilon/h_R = 1$ and -1, respectively.

the RH crystal and the LH crystal are weakly coupled and the two originally degenerate surface states split according to Eq. (21), and the bulk continuum part of $\rho_R(0)$ is predominantly R like as shown in Fig. 2(d). For $h_{RL}/h_R = 0.2$ [see Fig. 2(c)], the interface Shockley states split further apart and the bulk continuum part of $\rho_R(0)$ picks up some more L-like states. For $h_{RL}/h_R = 0.5$ [see Fig. 2(b)], the interface Shockley states merge into the bulk continuum and become resonance states, and, as a result, the bulk continuum is strongly enhanced. In addition, we also observe that the band-edge singularities associated with a perfect crystal are being washed out completely in $\rho_R(0)$. A similar kind of conclusion can be also drawn for $\rho_L(-1)$.

Symmetric case with $\gamma_R, \gamma_L < 1$. Here, both RH and LH crystals are band uncrossed, and thus there are no Shockley states in the gap region. However, we observe that, when $h_{RL} > h_R, h_L$ there exist two interface states in the outer band-edge regions as shown in Fig. 3. The set of parameters used here is $h_L/h_R = 1$, $\epsilon_R/h_L = \epsilon_L/h_R = 4$. The energies for the pair of interface states approach the limit of Eq. (22) as $h_{RL}/h_R \gg 1$.

Symmetric case of $\gamma_R > 1$ *and* $\gamma_L < 1$. In this case there is only one Shockley surface state associated with the RH crystal. As h_{RL} increases, the Shockley state will stay at $E = 0$, but will also decay into the LH crystal. The bulk continuum of $\rho_R(0)$ will also pick up more L-like states, as shown in Fig. 4.

Unsymmetric case with both γ_R *and* $\gamma_L > 1$. There are now two Shockley states at different energies. The energy of the Shockley state associated with the RH crystal lies in the continuum region of the LH crystal, and vice versa. As shown in Fig. 5,

one observes one resonance state and one dip in both $\rho_R(0)$ and $\rho_L(-1)$. This shows that the Shockley state associated with the RH crystal will not penetrate into the continuum of the LH crystal as a resonance state. The dashed lines describe the case of $h_{RL} = 0$.

Unsymmetric case with $\gamma_R > 1$ and $\gamma_L < 1$. In this case, the Shockley state associated with the LH crystal lies in the bulk continuum region of the RH crystal. In Fig. 6, one observes that the Shockley state which appears in $\rho_R(0)$ is broadened by coupling to the continuum, and a sharp dip appears in $\rho_L(-1)$ at the same energy where the Shockley state is located. This again shows that the Shockley state will not penetrate into the continuum of the other side of the interface.

IV. DISCUSSION

We have used the Green's-function method to study the electronic density of states at the interface of two semi-infinite one-dimensional lattices consisting of sp hybrid atoms. The interaction between two degenerate Shockley states and that between a Shockley state and a bulk continuum have received special attention. Our results indicate that a pair of degenerate Shockley states will split in the presence of a weak interface cou-

pling. They also reveal that the Shockley state will not penetrate into the bulk continuum as a resonance state, and, instead, there is a dip in the density of states at the energy of the Shockley state.

So far, only systems consisting of two pure semi-infinite one-dimensional lattices have been considered. No interface potential perturbation has been taken into account. However, this method is completely general, and can be applied to more complicated three-dimensional systems with some modification. Our calculation is essentially a one-electron theory for a static system. No attempt has been made to take into account the effect of the charge redistribution near the interface. Thus the phenomenon of band bending or a junction potential has been excluded from our discussion. Investigations on the effect of the charge redistribution have been reported in recent years by many authors[18,19]; however, they have left out the effect of the interface structure. A theory which includes both the effect of the charge redistribution and the effect of the crystal structure at the interface is needed in order to understand the nature of the electronic states at the interface. Our study of the "static" system is of some importance in the process of developing a more complete theory for the interface state.

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