

## Effective two-dimensional Hamiltonian at surfaces

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By means of decimation techniques as applied in the renormalization-group method, a new method is proposed to obtain the effective interactions for two-dimensional Hamiltonians at surfaces. The method has been applied to a simplified model of a transition metal and to Si. For the transition metal we recover well-known results as regards the general properties of the surface density of states, while for Si our results show that an effective two-dimensional Hamiltonian can be introduced along the line proposed by several authors, but with energy-dependent parameters.

### I. INTRODUCTION

In the last few years there has been a widespread interest in two-dimensional Hamiltonian models directed to the understanding of the mechanisms driving different semiconductor reconstructions.<sup>1-4</sup> The purpose of this approach is to circumvent the computational difficulties associated with a calculation of the whole three-dimensional structure.<sup>5,6</sup> In particular, simple two-dimensional Hamiltonians for Si surfaces have been proposed within a tight-binding approach, by introducing a nearest-neighbor interaction adjusted to give the appropriate dispersion relation for the surface band.

A very general discussion of two-dimensional effective Hamiltonians within a tight-binding approach can be given following the procedure of Lohez *et al.*<sup>7</sup> Consider the matrix equation for the Green function  $\underline{G}$ :

$$(\omega \underline{I} - \underline{H}) \underline{G} = \underline{I}, \quad (1)$$

where  $\omega$  is the energy and  $\underline{H}$  the Hamiltonian written in a given basis. Projecting Eq. (1) onto the two subspaces  $d$  and  $R$  associated with the dangling bonds we are interested in and with the rest of the whole space respectively, we obtain the following equations:

$$\begin{aligned} (\omega \underline{I}_{dd} - \underline{H}_{dd}) \underline{G}_{dd} + (-\underline{H}_{dR}) \underline{G}_{Rd} &= \underline{I}_{dd}, \\ (-\underline{H}_{Rd}) \underline{G}_{dd} + (\omega \underline{I}_{RR} - \underline{H}_{RR}) \underline{G}_{Rd} &= \underline{0}_{Rd}. \end{aligned} \quad (2)$$

By eliminating  $\underline{G}_{Rd}$  Eqs. (2) yield

$$(\omega \underline{I}_{dd} - \underline{H}_{dd} - \underline{\Sigma}_{dd}) \underline{G}_{dd} = \underline{I}_{dd}, \quad (3)$$

where the self-energy,  $\underline{\Sigma}_{dd}$ , is given by

$$\underline{\Sigma}_{dd} = -\underline{H}_{dR} (\omega \underline{I}_{RR} - \underline{H}_{RR})^{-1} \underline{H}_{Rd}. \quad (4)$$

Equation (3) looks like a two-dimensional Hamiltonian with effective interactions defined by the different Hamiltonian components  $\underline{H}_{dd}$ ,  $\underline{H}_{dR}$ , and  $\underline{H}_{RR}$ . The complex effective interaction,  $\underline{\Sigma}_{dd}$ , is dependent on the energy  $\omega$ , a fact introducing insurmountable problems for using Eq. (3) unless this  $\omega$  dependence is small or negligible within the region of interest. As a matter of fact that is what is expected to happen for the dangling-bond surface states of Si in the region of the optical gap.

The main purpose of this paper is to analyze the behavior of  $\underline{\Sigma}_{dd}$  for Si(111) surface, by means of a numerical procedure explained in Sec. II. By extension, we apply this procedure to the case of a simplified transition-metal surface and discuss the effective interactions for its reduced effective Hamiltonian.

In our procedure we introduce a small variance over the general method given above. Instead of working with the Green function in the real space, in a first step we work with a fixed momentum parallel to the surface ( $\vec{k}$ ), and look for the self-energy in the subspace of interest. This gives us  $\Sigma(\vec{k}, \omega)$  instead of  $\Sigma(\vec{R} - \vec{R}'; \omega)$ ; in a second step,  $\Sigma(\vec{R} - \vec{R}'; \omega)$  [or  $\Sigma_{dd}(\omega)$  in the previous notation] is obtained by an appropriate Fourier analysis.

In Sec. II we discuss the procedure used to obtain the self-energy. In Sec. III we present our results for the surface of a simplified model of a transition metal and for a Si(111) face. A final discussion of these results is also given in Sec. III.

### II. METHOD

In this section we start with Eq. (1) for the Green function  $\underline{G}$ , and write it in an appropriate basis

which we assume to be defined for our surface by a layer number  $m$ , an orbital index  $\alpha$ , and a momentum  $\vec{k}$ , parallel to the surface, belonging to the first Brillouin zone (BZ) of our two-dimensional surface lattice. Let us use  $a$  to denote the number of independent orbitals in each layer.

In this representation, a matrix element of, say, the Green function  $\underline{G}$ , takes the form  $G_{am,\alpha m'}(\vec{k})$ . In the following, instead of using this notation we shall write  $\underline{G}_{m,m'}(\vec{k})$ . or  $\underline{G}_{m,m'}(\vec{k}$  dependence understood), in such a way that an element  $(\alpha,\alpha')$  of

the matrix  $\underline{G}_{m,m'}(\vec{k})$  is  $G_{am,\alpha m'}(\vec{k})$ .

Now, we write Eq. (1) for  $\underline{G}$  in this representation by taking the elements  $(\alpha m, \alpha' 0)$  as follows:

$$\omega \underline{G}_{m,0} - \sum_{m'} \underline{H}_{m,m'} \underline{G}_{m',0} = \delta_{m,0}. \quad (5)$$

Let us now assume that the interaction between orbitals extend up to second-neighbor layers; with this particular case we try to show how to generalize the procedure to long-distance interactions. Then, Eq. (5) can be explicitly written as follows:

$$(\omega \underline{I}_{0,0} \underline{H}_{0,0}) \underline{G}_{0,0} - \underline{H}_{0,1} \underline{G}_{1,0} - \underline{H}_{0,2} \underline{G}_{2,0} = \underline{I}, \quad (6a)$$

$$-\underline{H}_{1,0} \underline{G}_{0,0} + (\omega \underline{I}_{1,1} - \underline{H}_{1,1}) \underline{G}_{1,0} - \underline{H}_{1,2} \underline{G}_{2,0} - \underline{H}_{1,3} \underline{G}_{3,0} = \underline{0}, \quad (6b)$$

$$-\underline{H}_{2,0} \underline{G}_{0,0} - \underline{H}_{2,1} \underline{G}_{1,0} + (\omega \underline{I}_{2,2} - \underline{H}_{2,2}) \underline{G}_{2,0} - \underline{H}_{2,3} \underline{G}_{3,0} - \underline{H}_{2,4} \underline{G}_{4,0} = \underline{0}, \quad (6c)$$

$$-\underline{H}_{m,m-2} \underline{G}_{m-2,0} - \underline{H}_{m,m-1} \underline{G}_{m-1,0} + (\omega - \underline{H}_{m,m}) \underline{G}_{m,0} - \underline{H}_{m,m+1} \underline{G}_{m+1,0} - \underline{H}_{m,m+2} \underline{G}_{m+2,0} = \underline{0}, \quad (6d)$$

where the different interactions between layers  $m$  and  $m'$  are given by  $\underline{H}_{m,m'}$ , and use has been made of the fact that interactions extend only up to second-neighbor layers. It is convenient to remark at this point that a layer, in the language used here, may be built up by several "crystal layers"; the number of crystal layers forming a layer is given by that number allowing us to write Hamiltonian (1), well inside the bulk,<sup>8</sup> in the form given by Eq. (6d).

For an ideal structure, we have

$$\underline{H}_{m,m'} = \underline{H}(m - m') \quad (7a)$$

and

$$H_{\alpha,\beta}(m - m') = H_{\beta,\alpha}^*(m' - m). \quad (7b)$$

For simplicity we limit our discussion to the case in which for the third layer [Eq. (6c)] we recover the general equation (6d). (In our second-neighbor approximation, this implies an ideal unrelaxed surface.) A more general case can be readily obtained. For the case of an ideal unrelaxed surface, Eq. (7a) can be used for all the matrix elements  $\underline{H}_{m,m'}$  appearing in Eqs. (6).

In the literature, these equations have been solved by the transfer-matrix method,<sup>9-11</sup> by reducing them to a finite system by taking a slab,<sup>12</sup> or by other methods.<sup>8</sup> In our procedure, we have followed decimation techniques as applied in the renormalization-group method.<sup>13</sup> The advantages of our procedure are its quick convergence and its saving of computer time.

It is now convenient to rewrite Eqs. (6) in the following way:

$$\begin{bmatrix} \omega \underline{I} - \underline{H}(0) & -\underline{H}(\bar{1}) \\ -\underline{H}(1) & \omega \underline{I} - \underline{H}(0) \end{bmatrix} \begin{bmatrix} \underline{G}_{0,0} \\ \underline{G}_{1,0} \end{bmatrix} + \begin{bmatrix} -\underline{H}(\bar{2}) & \underline{0} \\ -\underline{H}(\bar{1}) & -\underline{H}(\bar{2}) \end{bmatrix} \begin{bmatrix} \underline{G}_{2,0} \\ \underline{G}_{3,0} \end{bmatrix} = \begin{bmatrix} \underline{I} \\ \underline{0} \end{bmatrix} \quad (8)$$

$$\begin{bmatrix} -\underline{H}(2) & -\underline{H}(1) \\ \underline{0} & -\underline{H}(2) \end{bmatrix} \begin{bmatrix} \underline{G}_{m-2,0} \\ \underline{G}_{m-1,0} \end{bmatrix} + \begin{bmatrix} \omega \underline{I} - \underline{H}(0) & -\underline{H}(\bar{1}) \\ -\underline{H}(1) & \omega \underline{I} - \underline{H}(0) \end{bmatrix} \begin{bmatrix} \underline{G}_m \\ \underline{G}_{m+1} \end{bmatrix} + \begin{bmatrix} -\underline{H}(\bar{2}) & \underline{0} \\ -\underline{H}(\bar{1}) & -\underline{H}(\bar{2}) \end{bmatrix} \begin{bmatrix} \underline{G}_{m+2,0} \\ \underline{G}_{m+3,0} \end{bmatrix} = \underline{0}, \quad (9)$$

for  $m$  even, or equivalently, with an obvious notation,

$$\underline{W} \underline{G}_0 + \underline{I} \underline{G}_2 = \begin{bmatrix} \underline{I} \\ \underline{0} \end{bmatrix}, \quad (10a)$$

$$\underline{I}_2 \underline{G}_{m-2} + \underline{W} \underline{G}_m + \underline{I}_1 \underline{G}_{m+2} = \underline{0}. \quad (10b)$$

In these equations, 0,2,4, . . . , are the numbers associated to the different superlayers formed by the layers (0,1), (2,3), (4,5), and so on. Note that the number of layers defined inside each superlayer is related to the order of the interaction (second order here). According to decimation techniques, we proceed in successive steps by eliminating the even

Green functions associated to superlayers 2,6,10, . . . , in Eqs. (10). Thus in a first step we consider the following equations:

$$\tau_2 \mathcal{G}_0 + \underline{W} \mathcal{G}_2 + \tau_1 \mathcal{G}_4 = 0, \quad (11a)$$

$$\tau_2 \mathcal{G}_4 + \underline{W} \mathcal{G}_6 + \tau_1 \mathcal{G}_8 = 0, \quad (11b)$$

$$\tau_2 \mathcal{G}_8 + \underline{W} \mathcal{G}_{10} + \tau_1 \mathcal{G}_{12} = 0, \quad (11c)$$

and write

$$(\underline{W} - \tau_1 \underline{W}^{-1} \tau_2) \mathcal{G}_0 - (\tau_1 \underline{W}^{-1} \tau_1) \mathcal{G}_4 = \begin{bmatrix} I \\ 0 \end{bmatrix}, \quad (13a)$$

$$-(\tau_2 \underline{W}^{-1} \tau_2) \mathcal{G}_0 + (\underline{W} - \tau_2 \underline{W}^{-1} \tau_1 - \tau_1 \underline{W}^{-1} \tau_2) \mathcal{G}_4 - (\tau_1 \underline{W}^{-1} \tau_1) \mathcal{G}_8 = 0, \quad (13b)$$

$$-(\tau_2 \underline{W}^{-1} \tau_2) \mathcal{G}_4 + (\underline{W} - \tau_2 \underline{W}^{-1} \tau_1 - \tau_1 \underline{W}^{-1} \tau_2) \mathcal{G}_8 - (\tau_1 \underline{W}^{-1} \tau_1) \mathcal{G}_{12} = 0. \quad (13c)$$

These equations coincide with Eqs. (10) by an appropriate renormalization of the different matrices. Thus with the following definitions:

$$\underline{W}'_s = \underline{W} - \tau_1 \underline{W}^{-1} \tau_2, \quad (14a)$$

$$\underline{W}'_b = \underline{W} - \tau_1 \underline{W}^{-1} \tau_2 - \tau_2 \underline{W}^{-1} \tau_1, \quad (14b)$$

$$\tau'_1 = -\tau_1 \underline{W}^{-1} \tau_1, \quad (14c)$$

$$\tau'_2 = -\tau_2 \underline{W}^{-1} \tau_2, \quad (14d)$$

we recover formally Eqs. (10) with new renormalized parameters. For instance,  $\tau'_1$  and  $\tau'_2$  measure the effective interaction between renormalized superlayers 0 and 4, 4 and 8, and so on, while  $(\underline{W} - \tau_1 \underline{W}^{-1} \tau_2)$  can be defined as the effective matrix of  $(\omega - \underline{H})$  for layer 0 and  $(\underline{W} - \tau_1 \underline{W}^{-1} \tau_2 - \tau_2 \underline{W}^{-1} \tau_1)$  the same effective matrix for superlayers 4, 8, . . . .

Now, the procedure can be iterated, and at any step, say  $p$ , we obtain the following matrices as a function of the ones obtained in step  $(p-1)$ :

$$\underline{W}_s^{(p)} = \underline{W}_s^{(p-1)} - \tau_1^{(p-1)} (\underline{W}_b^{(p-1)})^{-1} \tau_2^{(p-1)}, \quad (15a)$$

$$\underline{W}_b^{(p)} = \underline{W}_b^{(p-1)} - \tau_1^{(p-1)} (\underline{W}_b^{(p-1)})^{-1} \tau_2^{(p-1)} - \tau_2^{(p-1)} [\underline{W}_b^{(p-1)}]^{-1} \tau_1^{(p-1)}, \quad (15b)$$

$$\tau_1^{(p)} = -\tau_1^{(p-1)} [\underline{W}_b^{(p-1)}]^{-1} \tau_1^{(p-1)}, \quad (15c)$$

$$\tau_2^{(p)} = -\tau_2^{(p-1)} [\underline{W}_b^{(p-1)}]^{-1} \tau_2^{(p-1)}. \quad (15d)$$

Note that for the second step,  $\tau_1^{(2)}$  and  $\tau_2^{(2)}$  give the effective interaction between renormalized superlayers 0 and 8, 8 and 16, and so on, while  $\tau_1^{(3)}$  and  $\tau_2^{(3)}$  measure the effective interaction for superlayers 0 and 16, 16 and 32, etc. In general, after  $p$  steps,  $\tau_1^{(p)}$  and  $\tau_2^{(p)}$  give the effective interaction between superlayers 0 and  $2^{p+1}$ , having renormalized out  $2^p$  superlayers. This is the important point of the procedure followed in this paper, since the num-

$$\mathcal{G}_2 = -\underline{W}^{-1} (\tau_2 \mathcal{G}_0 + \tau_1 \mathcal{G}_4), \quad (12a)$$

$$\mathcal{G}_6 = -\underline{W}^{-1} (\tau_2 \mathcal{G}_4 + \tau_1 \mathcal{G}_8), \quad (12b)$$

$$\mathcal{G}_{10} = -\underline{W}^{-1} (\tau_2 \mathcal{G}_8 + \tau_1 \mathcal{G}_{12}). \quad (12c)$$

Now these equations are used to eliminate  $\mathcal{G}_2, \mathcal{G}_6, \mathcal{G}_{10}, \dots$ , from Eqs. (10). This procedure yields

ber of renormalized superlayers grows with an exponential power of the number of steps. On the other hand, we can expect both  $\tau_1^{(p)}$  and  $\tau_2^{(p)}$  to decrease, for any value of  $\omega$ , with the increasing number of steps; this is a conclusion that can be reached on physical grounds by noting that the effective interaction between superlayers must be small when they are far apart. Let us assume that, after  $p_0$  steps,  $\tau_1^{(p_0)}$  and  $\tau_2^{(p_0)}$  are negligible. Then, Eqs. (13) reduce to

$$\underline{W}_s^{(p_0)} \mathcal{G}_0 = \begin{bmatrix} I \\ 0 \end{bmatrix}, \quad (16a)$$

$$\underline{W}_b^{(p_0)} \mathcal{G}_{(2^{p_0+1})} = 0. \quad (16b)$$

It is obvious from Eqs. (15) that when  $\tau_1^{(p_0)}$  and  $\tau_2^{(p_0)}$  are small enough, a new step produces no change on the values of  $\underline{W}_s^{(p_0)}$  and  $\underline{W}_b^{(p_0)}$ ; the physical meaning of this result is clear: the surface and bulk superlayers are practically decoupled. Then,  $\underline{W}_s^{(p_0)}$  and  $\underline{W}_b^{(p_0)}$  give the effective matrices of  $(\omega - \underline{H})$ , for the surface and bulk superlayers, respectively.

In practical terms,  $\tau_1^{(p)}$  and  $\tau_2^{(p)}$  become small as a function of the chosen degree of accuracy for our effective Hamiltonians. Accordingly, we neglect  $\tau_1^{(p_0)}$  and  $\tau_2^{(p_0)}$  when, for step  $(p_0+1)$ , the differences between the values of every term of  $\underline{W}_s^{(p_0)}$  (or  $\underline{W}_b^{(p_0)}$ ) and  $\underline{W}_s^{(p_0+1)}$  (or  $\underline{W}_b^{(p_0+1)}$ ) are smaller than a given number, for any frequency. This is equivalent to say that, to a given accuracy, a slab of  $2^{p_0}$  superlayers is large enough to decouple both surfaces. Note that our results, after  $p_0$  steps, are equivalent to the ones given by the matrix-transfer method after  $2^{p_0}$  steps.

$\underline{W}_s^{(p_0)}$  and  $\underline{W}_b^{(p_0)}$  give the effective Hamiltonians for the isolated surface and bulk superlayers, respectively, and allows us to obtain, for instance, the den-

sity of states not only for the surface but for the bulk, too. As regards  $\underline{W}_s^{(p_0)}$ , this matrix gives an effective Hamiltonian in a basis which includes not only the dangling-bond orbital, but the  $2a$  orbitals associated to the last two layers. A final step must be given if we are interested in obtaining the effective two-dimensional Hamiltonian associated, say, to the dangling bonds of a Si(111) face. In this case, we eliminate from Eq. (16a) all the terms associated to  $\underline{G}_{0,0}$  and  $\underline{G}_{1,0}$ , except those related to the dangling-bond orbital. For the case of Si(111) (see below), this amounts to renormalizing out seven orbitals of the last surface layer. This final step gives  $(\omega \underline{I}_{dd} - \underline{H}_{dd,\text{eff}})$  where  $\underline{H}_{dd,\text{eff}}$  is the effective Hamiltonian associated to the dangling-bond orbitals, for a given momentum  $\vec{\kappa}$  parallel to the surface. Once that  $\underline{H}_{dd,\text{eff}}(\vec{\kappa}, \omega)$  has been obtained, we get the effective interactions for the dangling bonds by means of the following equation:

$$\underline{H}_{dd,\text{eff}}(\omega, \vec{\mathbf{R}}) = \sum_{\text{BZ}} \underline{H}_{dd,\text{eff}}(\omega, \vec{\kappa}) e^{i\vec{\kappa} \cdot \vec{\mathbf{R}}} . \quad (17)$$

### III. RESULTS: TRANSITION METALS AND Si

In this section we apply the method given above to getting the effective two-dimensional Hamiltonian for the surfaces of a simplified model of transition metal and Si.

#### A. Transition metal

In this case, we consider a (111) surface of a simplified transition metal with only two hybridized bands ( $s$  and  $d$ ), and a fcc structure. For this model we follow Harrison,<sup>14</sup> and define the transition-metal structure by means of the following parame-

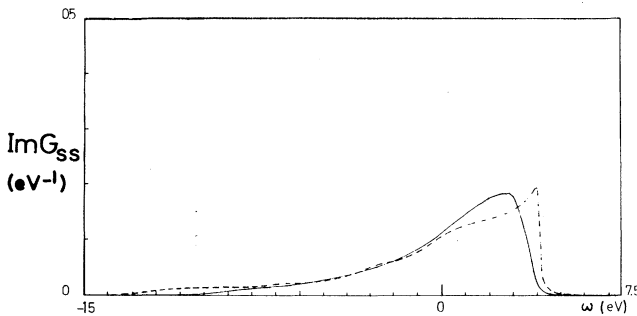


FIG. 1. Bulk (dashed line) and the surface (full line) density of states ( $\pi^{-1} \text{Im}G_{ss}$ ) for the  $s$  band of a simplified model of transition metal (see text).

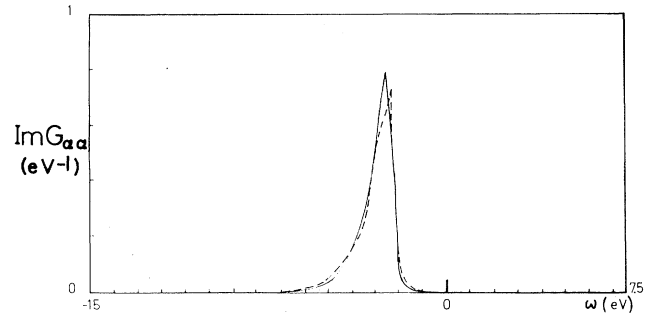


FIG. 2. Same as in Fig. 1 for the  $d$  band.

ters (measured in eV):

$$\epsilon_s = 0, \quad \epsilon_d = -3$$

$$V_{ss} = -1, \quad V_{sd} = -0.2, \quad V_{dd} = -0.25,$$

where  $\epsilon_s$  and  $\epsilon_d$  are the mean levels for the  $s$  and  $d$  bands, and  $V_{ss}$ ,  $V_{sd}$ , and  $V_{dd}$  are the interaction parameters for the different first-neighbor orbitals. In this model we neglect second-neighbor and further interactions.

With this simple first-neighbor interaction model, we can simplify the analysis given in Sec. II. In particular, instead of defining superlayers by two layers, we can now identify a superlayer with a layer and even with a "crystal layer." This allows us to reduce the dimensions of the matrix Green function,  $\underline{G}$ , to the number of orbitals per atom, namely, two. In the same way,  $\underline{W}_s^{(p_0)}$  and  $\underline{W}_b^{(p_0)}$  reduce to square matrices of  $2 \times 2$ , giving the effective Hamiltonians for the surface and the bulk layers. The first matrix defines the effective surface Hamiltonian we are looking for.

One word of caution must be put here. As is well known, in all the matrix-transfer methods a finite broadening must be introduced in the energy in order to get meaningful results. This amounts to substituting  $\omega$  by  $\omega + i\delta$ , where  $\delta$  is a quantity related to

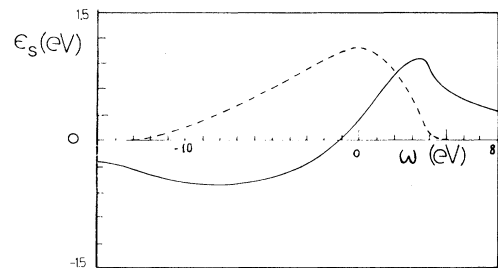


FIG. 3. Real (full line) and imaginary (dashed line) values of  $\epsilon_s$  as a function of  $\omega$ , for the surface of a simplified model of transition metal.

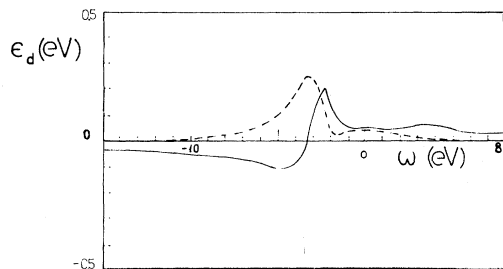


FIG. 4. Same as in Fig. 3 for  $\epsilon_d$  [ $\delta\epsilon_d = \epsilon_d(\omega) + 3$  eV].

the degree of accuracy accepted for the calculation. In our case, we have taken  $\delta = 0.05$  eV, in such a way that the accuracy of our results can be expected to be better than 0.1 eV. On the other hand, in order to get the same accuracy in the matrices  $\underline{W}_s^{(p_0)}$  and  $\underline{W}_b^{(p_0)}$ , we have to give six steps ( $p_0 = 6$ ). Finally, Eq. (17) has been applied to the present case by taking 45 points in the irreducible part of the two-dimensional BZ.<sup>15</sup>

We show our results in Figs. 1–6. In Fig. 1 (and Fig. 2) we give the surface and bulk density of states for the  $s$  (and  $d$ ) band. Note the small narrowing of the surface density of states, a well-known effect.<sup>16</sup> In Figs. 3–5 we give the effective values of  $\epsilon_s$ ,  $\epsilon_d$ , and  $V_{ss}$  as a function of  $\omega$ . Note the changes appearing in the effective interaction  $V_{ss}$ ; they are not greater than 30%, and their effect is to decrease the absolute value of  $V_{ss}$  inside the band, this fact being related to the narrowing of the surface density of states.

Another interesting fact of our results is that the effective interactions for second (and further) neighbors are rather small. This is shown in Fig. 6, where  $V_{ss}$  is drawn as a function of  $\omega$  for first, second, third, and fourth neighbors.

The general conclusion of our results for the simplified model of transition metal we have analyzed, is that the effective interactions for the surface layer are not far from the ideal bulk interactions. This suggests that even a monolayer of a metal may qualitatively reproduce properties of the surface of a

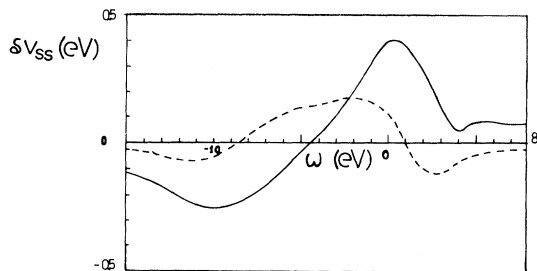


FIG. 5. Same as in Fig. 3 for  $V_{ss}$  [ $\delta V_{ss} = V_{ss}(\omega) + 1$  eV].

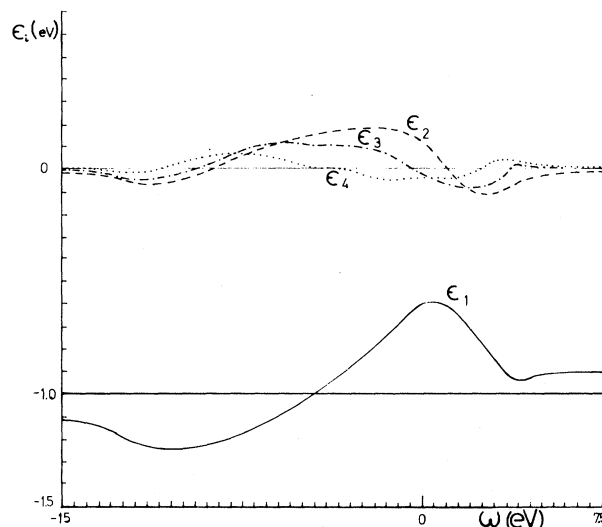


FIG. 6. Same as in Fig. 3 for the first-, second-, third-, and fourth-neighbor interactions (only the real part has been shown).

semi-infinite crystal. In particular, we can expect the height barrier of a metal-semiconductor junction to be practically formed with only a metal monolayer.

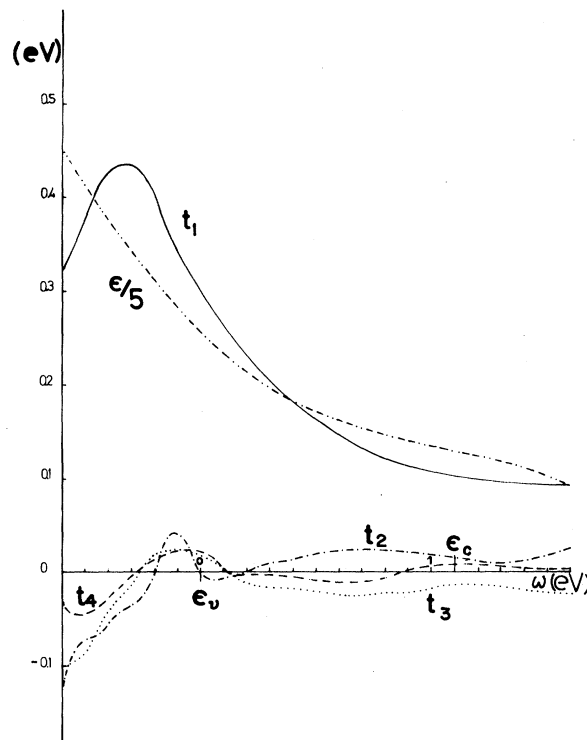


FIG. 7. Real part of the effective hybrid level  $\epsilon$  and the effective interaction  $t$  between dangling bonds up to the fourth neighbor for the Si(111) face.

### B. Si(111) surface

For Si we have considered the 111 surface of a tight-binding model with Koster-Slater parameters, having interactions between the different orbitals extending up to second neighbors. In this case, we have defined a layer by two "crystal layers," with interactions extending up to nearest-neighbors layers. Other details of interest are the following:  $\delta$  (see Sec. III A) has been taken to be 0.05 eV; the number of steps to get convergence has again been six and the number of points used in the irreducible two-dimensional BZ has been 45 as well.

The main results of our calculation are given in Fig. 7, where we show the real part of the effective hybrid level  $\epsilon$ , and the effective interactions between dangling bonds extending up to the fourth neighbor. The important result is that the interactions for the second—and further—neighbors are negligible (as well as all the imaginary components not given in the figure) in the region around the main gap. Our results show that an effective two-dimensional Ham-

iltonian with only two parameters,  $\epsilon$  and  $t_1$ , is a good approximation for analyzing the surface band. However, *these two parameters cannot be taken as constants*. According to our analysis, an appropriate two-dimensional Hamiltonian for the Si(111) surface must include in the parameters  $\epsilon$  and  $t_1$  at least a linear dependence on  $\omega$ . Note that the values given in Fig. 7 are consistent with a surface band located just below the valence-band edge  $\epsilon_v$  in good agreement with the results of Pandey and Phillips<sup>12</sup> (the hybrid  $sp^3$  level is around 1.3 eV below  $\epsilon_v$ ). We stress that the two-dimensional effective Hamiltonian is only useful near the main gap; for instance, surface resonances could be only analyzed in practice by means of the whole three-dimensional decimation technique.

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