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Electronic structure of line defects by means of the scattering theoretical method. Application to lines of vacancies in the simple cubic lattice

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The scattering theoretical method recently used to describe the electronic structure of point defects in solids is extended to study line defects. The method is applied to the case of lines of vacancies in the simple cubic lattice within a tight-binding model. Lines of vacancies in the [100], [110], and [111] directions are considered, and their formation energies are estimated within the independent-electron approximation. The interaction energy between parallel lines of vacancies is also studied and the results are compared with those obtained for the interaction energy between single vacancies; both interaction energies are shown to be remarkably similar.

I. INTRODUCTION

In the last few years there has been a strong revival of interest in the electronic properties of defects in solids.[1–17] Point defects, such as vacancies, have been studied in the bulk, surfaces, and interfaces of both metals and semiconductors.[1–14] On the other hand, line defects, such as dislocations, have received little attention.[15–17] This is mainly due to the following: (i) the most dramatic effect of dislocations is to be found in the mechanical properties of solids; therefore these properties have attracted most interest, and (ii) the difficulties in treating the severe breaking of symmetry introduced by line defects. Nowadays it is generally recognized that, as do point defects, line defects should dramatically affect the electronic properties of solids and may play a fundamental role in determining such an important property as the catalytic activity of metal surfaces. Recently, there have been several attempts to extend the methods of calculation used to study surfaces and vacancies to the case of line defects.[15–17] Those analyses have always treated line defects by means of superlattice methods.

The purpose of the present work is to show how the scattering theoretical method recently used to describe the electronic structure of surfaces, interfaces, and point defects in solids can be extended to treat simple line defects. In particular, we shall discuss its application to the case of lines of vacancies in the three main directions of the simple-cubic lattice. The formation energies of lines of vacancies (the difference between the energy of a crystal containing a line of N vacancies and the energy of a crystal with N isolated vacancies) will be estimated in the independent electron approximation, and the interaction between parallel lines of vacancies will be studied in the same approximation. Our results will be compared with those obtained by Yaniv[13,14] for the case of single vacancies. Of course, and due to the approximate nature of the model Hamiltonian (simple cubic lattice, one orbital per site, interactions up to first neighbors, neglect of the electron-electron and ion-ion interactions, and absence of ionic relaxations), our emphasis will be on the techniques required by the extension of the scattering method to handle line defects, but not on the study of a realistic situation.

II. METHOD OF CALCULATION

The formalism we shall use is based upon the Green's-function method. The single-particle Green's function associated with a given Hamiltonian H_0 is given by

$$(E+i\eta-H_0)G_0=1\ , \tag{1}$$

E being the energy and η a positive infinitesimal. The vacancy or line of vacancies is introduced through a localized perturbation V. The perturbed Schrödinger equation is now written as

$$H\,|\,\psi\rangle=(H_0+V)\,|\,\psi\rangle=E\,|\,\psi\rangle\ . \tag{2}$$

The perturbed Green's function is then given by Dyson's equation, namely,

$$G=G_0+G_0VG\ . \tag{3}$$

The phase shift associated with this scattering problem is given by

$$\delta(E)=\arg[D(E)]\ . \tag{4}$$

where $D(E)$ is obtained through

$$D(E)=\det(1-G_0V)\ . \tag{5}$$

Finally, the change in the density of states caused by the localized perturbation V is written as

$$\Delta N(E)=-\frac{1}{\pi}\frac{\partial}{\partial E}\delta(E)\ . \tag{6}$$

In the present work we shall consider a simple single-state Hamiltonian, which in the site representation takes the form

$$H_0=\sum_{i,j}h_{ij}\,|\,\vec{\mathrm{i}}\,\rangle\langle\,\vec{\mathrm{j}}\,|\ . \tag{7}$$

i and j run over the lattice sites and h_{ij} is restricted to nearest-neighbor interactions, namely $h_{ij}=h_0$ if i and j are nearest neighbors and zero otherwise.

Now, if a vacancy is created at a lattice site $\vec{m}$, the localized potential can be written as

$$V_{\vec{m}} = V_0 |\vec{m}\rangle\langle\vec{m}| . \tag{8}$$

To treat this vacancy problem we can use a simple method[6,9,13] that greatly simplifies the calculations, namely, we let V_0 tend to infinity. In this way (4) can be rewritten as

$$\delta_{\vec{m}}(E) = \arg[G_0(\vec{m},\vec{m})] . \tag{9}$$

Here we note that with the simple Hamiltonian of Eq. (7) the Green's function is no longer a matrix, but a scalar. Therefore $\Delta N(E)$ is directly obtained from the unperturbed Green's function calculated at the site where the vacancy has been created.

This method also allows us to study the interaction between two vacancies.[13] In this case the localized potential is written as

$$V_{\vec{m},\vec{n}} = V_0 (|\vec{m}\rangle\langle\vec{m}| + |\vec{n}\rangle\langle\vec{n}|) . \tag{10}$$

The phase shift associated with this potential is given by

$$\begin{aligned}\delta_{\vec{m},\vec{n}}(E) = \arg[&G_0(\vec{m},\vec{m})G_0(\vec{n},\vec{n}) \\ &- G_0(\vec{m},\vec{n})G_0(\vec{n},\vec{m})] .\end{aligned} \tag{11}$$

If the two vacancies were noninteracting, the phase shift would be

$$\delta^0_{\vec{m},\vec{n}}(E) = \arg[G_0(\vec{m},\vec{m})G_0(\vec{n},\vec{n})] . \tag{12}$$

Therefore the increment in the phase shift due to vacancy-vacancy interaction is given by

$$\begin{aligned}\Delta\delta_{\vec{m},\vec{n}}(E) &= \delta_{\vec{m},\vec{n}}(E) - \delta^0_{\vec{m},\vec{n}}(E) \\ &= \arg\left[1 - \frac{G_0(\vec{m},\vec{n})G_0(\vec{n},\vec{m})}{G_0(\vec{m},\vec{m})G_0(\vec{n},\vec{n})}\right] .\end{aligned} \tag{13}$$

This allows us to calculate the vacancy-vacancy interaction energy in the independent electron approximation.[18] The interaction energy is written as

$$E_{\vec{m},\vec{n}} = \int_{-\infty}^{E_F} [\Delta N_{\vec{m},\vec{n}}(E) - \Delta N^0_{\vec{m},\vec{n}}(E)] E \, dE . \tag{14}$$

This equation can be written by using Eqs. (6) and (13) and integrating by parts:

$$E_{\vec{m},\vec{n}} = \pi^{-1} \int_{-\infty}^{E_F} [\delta_{\vec{m},\vec{n}}(E) - \delta^0_{\vec{m},\vec{n}}(E)] dE . \tag{15}$$

Note that Eq. (15) is usually valid if the number of electrons of the perturbed system equals the number of electrons of the unperturbed system. Neither the system with two noninteracting vacancies nor the system with two interacting vacancies holds normally the same number of electrons as the unperturbed system. Nevertheless, Eq. (15) is applicable if the number of electrons of both perturbed systems is supposed to be the same. We do assume this situation.

Equation (15) together with Eqs. (6)–(9) fully define our system for the case of single vacancies. We turn now to consider the case of lines of vacancies.

The extension of the formalism described above to the case of lines of vacancies (LV) is as follows. A line of vacancies along the direction $\hat{u}$ is a set of vacancies separated by a vector $\vec{R}$ ($\vec{R} \| \hat{u}$) that belongs to the three-dimensional direct lattice and is the shortest vector in this direction. Therefore, the localized potential of the LV is given by

$$V^1_{\mathrm{LV}} = V_0 \sum_{j=-\infty}^{\infty} |\vec{m} + j\vec{R}\rangle\langle\vec{m} + j\vec{R}| . \tag{16}$$

Once the LV is created the only symmetry that remains is the translational symmetry along the direction of the line defect and with a periodicity $\vec{R}$. Therefore the most convenient representation to study the LV is a mixed one: The spatial coordinate along the direction of the line defect is Fourier-transformed, whereas the position representation in the plane perpendicular to the line defect is retained. We denote the wave vector along the direction of the line defect by k and the origin of a generic line of atoms parallel to the LV by $\vec{\sigma}$. The wave vector k runs over the one-dimensional Brillouin zone (1DBZ), i.e., $-\pi/R \le k \le \pi/R$. The knowledge of the set of lattice positions over which $\vec{\sigma}$ runs requires an adequate geometrical decomposition of the crystal lattice. The three-dimensional Bravais lattice is decomposed into a family of lattice planes perpendicular to the LV and characterized by a vector $\vec{G}$ of the three-dimensional reciprocal lattice (Aschroft and Mermin, Ref. 18, p. 90). Those lattice planes are separated by a distance $d = 2\pi/G$, generally shorter than R. Actually,

$$\vec{G} \cdot \vec{R} = GR = 2\pi n, \; n \ge 1 \tag{17}$$

implies

$$d = \frac{2\pi}{G} = \frac{R}{n} . \tag{18}$$

It follows from the preceding discussion that the two-dimensional vector $\vec{\sigma}$ gives the projection in a plane perpendicular to the line defect of the atoms in $n = R/d$ lattice planes. In other words, $\vec{\sigma}$ does not describe a two-dimensional Bravais lattice if n is greater than 1. For example, n is equal to 1, 2, and 3 for the LV in the [100], [110], and [111] directions, respectively.

This peculiar geometrical situation must be carefully taken into account in the computation of the Green's function in the mixed representation $(\vec{\sigma},k)$. In fact, we start from the Green's function in a three-dimensional wave-vector representation $\vec{k}$ ($\vec{k} \in$ 3DBZ), in which the Green's function is diagonal. In a second step, we construct the two-dimensional Brillouin zone (2DBZ) corresponding to the Bravais lattice defined by a lattice plane perpendicular to the LV. Finally, we integrate the Green's function over the 2DBZ to transform it into the position representation $\vec{\sigma}$. The possibility of such a constructive process rests on the fact that the original three-dimensional reciprocal lattice is always transformable into a three-dimensional reciprocal lattice whose 3DBZ is a right prism. The basis of the right prism is the 2DBZ, and the following relationship holds:

$$\frac{\Omega_{3\mathrm{D}}(\text{original})}{\Omega_{3\mathrm{D}}(\text{new})} = n , \tag{19}$$

where Ω_{3D} is the volume of the 3DBZ. This is the reciprocal-space formulation of the real-space decomposition into lattice planes discussed above.

Once the pertinent entities are defined we can proceed further. The Green's function in the mixed representation is given by

$$G_0(k,\vec{\sigma}_1;k,\vec{\sigma}_2)=\sum_{\vec{q}\in 2\mathrm{DBZ}} e^{i\vec{q}\cdot(\vec{\sigma}_1-\vec{\sigma}_2)}G_0(k,\vec{q})\ . \tag{20}$$

The potential V_{LV}^1 is Fourier-transformed along the direction of the LV and yields

$$V_{\mathrm{LV}}^1=V_0\sum_{k\in 1\mathrm{DBZ}}|k,\vec{\sigma}_v\rangle\langle k,\vec{\sigma}_v|\ , \tag{21}$$

$\vec{\sigma}_v$ being the origin of the LV. The elements of the Fredholm determinant [Eq. (5)] are

$$\begin{aligned}\langle k_1,\vec{\sigma}_1|(1-G_0V_{\mathrm{LV}}^1)|k_2,\vec{\sigma}_2\rangle &=\delta_{k_1k_2}\delta_{\vec{\sigma}_1\vec{\sigma}_2}-\sum_{k_3,\vec{\sigma}_3}G_0(k_1,\vec{\sigma}_1;k_3,\vec{\sigma}_3)\langle k_3,\vec{\sigma}_3|V_{\mathrm{LV}}^1|k_2,\vec{\sigma}_2\rangle\\ &=\delta_{k_1k_2}[\delta_{\vec{\sigma}_1\vec{\sigma}_2}-V_0\delta_{\vec{\sigma}_2\vec{\sigma}_v}G_0(k_1\vec{\sigma}_1;k_1\vec{\sigma}_v)]\ ,\end{aligned} \tag{22}$$

where the diagonality of G_0 in the k index has been used. This is the crucial point in the whole theory: The Fredholm determinant factorizes in the wave-vector index k. It allows one to obtain the phase shift originated by the defect:

$$\begin{aligned}\delta_{\mathrm{LV}}^1(E)&=\arg\det(1-G_0V_{\mathrm{LV}}^1)\\ &=\arg\prod_{k\in 1\mathrm{DBZ}}[1-V_0G_0(k,\vec{\sigma}_v;k,\vec{\sigma}_v)]\\ &=\sum_{k\in 1\mathrm{DBZ}}\arg[1-V_0G_0(k,\vec{\sigma}_v;k,\vec{\sigma}_v)]\ ,\end{aligned} \tag{23}$$

which yields in the limit $V_0\rightarrow\infty$,

$$\delta_{\mathrm{LV}}^1(E)=\sum_{k\in 1\mathrm{DBZ}}\arg G_0(k,\vec{\sigma}_v;k,\vec{\sigma}_v)\ . \tag{24}$$

Therefore the phase shift associated with a LV can be calculated as easily as that corresponding to a single vacancy. Similarly we may write the potential associated with two parallel LV, namely

$$V_{\mathrm{LV}}^2=V_0\sum_{j=-\infty}^{\infty}(|\vec{m}+j\vec{R}\rangle\langle\vec{m}+j\vec{R}|+|\vec{n}+j\vec{R}\rangle\langle\vec{n}+j\vec{R}|)\ . \tag{25}$$

In this case the change in the phase shift due to the interaction between LV is given by

$$\Delta\delta_{\mathrm{LV}}^2(E)=\sum_{k\in 1\mathrm{DBZ}}\arg\left[1-\frac{G_0(k,\vec{\sigma}_v;k,\vec{\sigma}\,'_v)G_0(k,\vec{\sigma}\,'_v;k,\vec{\sigma}_v)}{G_0(k,\vec{\sigma}_v;k,\vec{\sigma}_v)G_0(k,\vec{\sigma}\,'_v;k,\vec{\sigma}\,'_v)}\right]\ , \tag{26}$$

where $\vec{\sigma}_v$ and $\vec{\sigma}\,'_v$ are the origins of the two LV. By introducing this expression in Eq. (15) we may calculate the interaction energy between two parallel LV.

The above formalism can also be applied to the study of dislocations if situations in which the Burgers vectors add to zero are studied.[19] This requisite also applies to the superlattice method,[16] but whereas within the present formalism a finite set of dislocations may be studied, within the superlattice method a periodic repetition of a finite set of dislocations is solved. As an example of the power of the Green's-function method the phase shift produced by two edge dislocations along the [100] direction in the simple cubic (sc) lattice and with opposite Burgers vectors is given in an appendix. In this paper we have not further applied the scattering theoretical method to the study of dislocations.

III. LV IN THE sc LATTICE

In this section we shall present our results for LV in the three main directions of the cubic lattice. We first concentrate on a single LV. To use the formalism presented in the preceding section, we must calculate the Green's function of the cubic lattice. A thorough discussion of the properties and the method for calculating the Green's function of the cubic lattice can be found in Ref. 20. Here we shall briefly discuss a few points relevant to the present work. In particular, we are interested in calculating the Green's function as a function of the component of the crystal momentum in the direction of the LV. This can be written as

$$G(\phi_1,m_2,m_3;\phi_1,n_2,n_3)=\frac{1}{(b_2-a_2)(b_3-a_3)}\int_{a_2}^{b_2}d\phi_2\int_{a_3}^{b_3}d\phi_3\frac{e^{i[\phi_2(m_2-n_2)+\phi_3(m_3-n_3)]}}{z-f(\phi_1,\phi_2,\phi_3)}\ , \tag{27}$$

where $\vec{\phi}=a\vec{k}$, $\vec{k}$ being the crystal momentum; note that ϕ_1 is the component in the direction of the line of vacancies. z is $\epsilon+i\eta$, ϵ being the energy referred to the energy of the s orbital and η a positive infinitesimal, f is a function of the three components of $\vec{\phi}$, and a_i,b_i, $i=2,3$ are the integration limits. The function f and a_i and b_i actually depend on the direction we are concerned with. Equation (27) can be rewritten in a more convenient way for the three main directions of the cubic lattice:

$$G(\phi_1,m_2,m_3;\phi_1,n_2,n_3)=\frac{1}{(b_2-a_2)(b_3-a_3)}\int_{a_2}^{b_2}d\phi_2\int_{a_3}^{b_3}d\phi_3\frac{e^{i[\phi_2(m_2-n_2)+\phi_3(m_3-n_3)]}}{E-B\cos(b\phi_3)} \tag{28}$$

where $E=z-f_1(\phi_1,\phi_2)$ and $B=f_2(\phi_1,\phi_2)$. Both f_1 and f_2 and the constant b depend on the actual crystal direction. This double integral can be easily calculated for the [100] direction (see Chap. 5 of Ref. 20), and for the other two directions, i.e., [110] and [111], one of the integrals (ϕ_3) can be solved analytically and the other must be solved numerically.

The values of the different functions and parameters for the three main directions are as follows. For the [100] direction we have

$$f_1=2h_0(\cos\phi_1+\cos\phi_2)\ ,\quad f_2=2h_0\ ,\quad b=1\ , \tag{29}$$

and the three components of $\vec{\phi}$ vary in the following intervals:

$$-\pi\le\phi_1\le\pi\ ,\quad -\pi\le\phi_2\le\pi\ ,\quad -\pi\le\phi_3\le\pi\ .$$

For the (110) direction we obtain

$$f_1=2h_0\cos\phi_2\ ,\quad f_2=4h_0\cos\phi_1\ ,\quad b=1/\sqrt{2}\ , \tag{30}$$

and

$$-(\sqrt{2}/2)\pi\le\phi_1\le(\sqrt{2}/2)\pi\ ,$$
$$-\pi\le\phi_2\le\pi\ ,$$
$$-\sqrt{2}\pi\le\phi_3\le\sqrt{2}\pi\ .$$

Finally, for the [111] direction the functions are

$$f_1=2h_0\cos[(\sqrt{2}\phi_2-\phi_1)/\sqrt{3}]\ ,$$
$$f_2=4h_0\cos[(\phi_1+\phi_2/\sqrt{2})/\sqrt{3}]\ , \tag{31}$$
$$b=1/\sqrt{2}\ ,$$

and

$$-\pi/\sqrt{3}\le\phi_1\le\pi/\sqrt{3}\ ,$$
$$-2\sqrt{2/3}\pi\le\phi_2\le2\sqrt{2/3}\pi\ ,$$
$$-\sqrt{2}\pi\le\phi_3\le\sqrt{2}\pi\ .$$

Here we note that in order to evaluate the ϕ_3 integral analytically we integrate in a rectangular zone larger than the actual zone (a regular hexagon).

Once we have calculated the Green's functions, the application of the formalism described in the preceding sec-

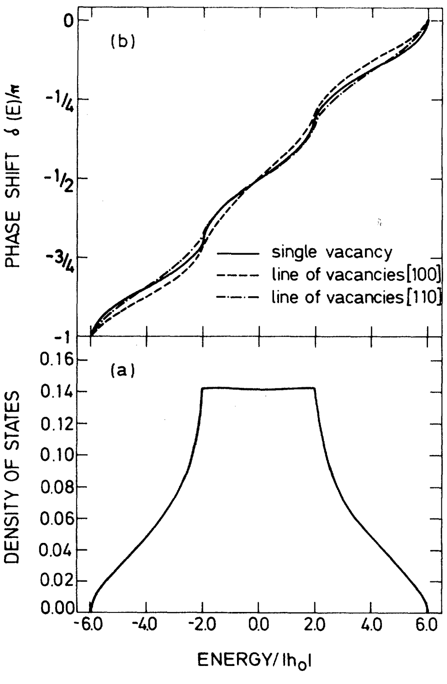

FIG. 1. (a) Local density of states (normalized to one state per spin) at a bulk atom in the sc lattice obtained by means of a one-state (s-like) Hamiltonian. (b) Phase shift per spin [$\delta(E)$ defined in Eq. (4)] of a bulk vacancy (solid line), and of a LV in the [100] direction [in this case $\delta(E)$ is per spin and per atom] dashed line) and in the [100] direction (dashed-dotted line). The energy is referred to the nearest-neighbor interaction h_0.

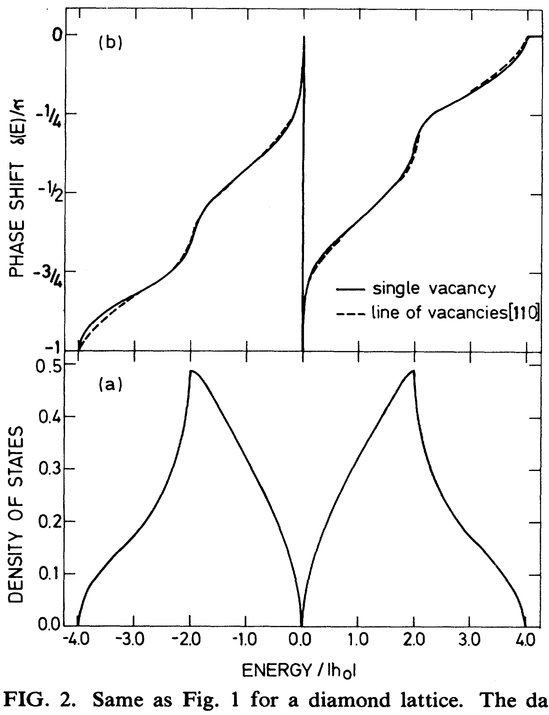

FIG. 2. Same as Fig. 1 for a diamond lattice. The dashed line in (b) corresponds to a LV in the [110] direction.

tion to the present case is straightforward. First we describe our results for isolated LV. Our results for the phase shifts per spin for a single vacancy and for LV in the [100] and [110] directions are shown in Fig. 1. In the case of LV, $\delta(E)$ is also normalized to one atom. The phase shift for a LV in the [111] direction is not shown for the sake of clarity. We note that although the phase shift corresponding to LV significantly differs from that of an isolated vacancy, no qualitative changes are found. To further illustrate this point, we consider the case of a more structured lattice, namely, the diamond lattice; again we use a single-state Hamiltonian. In Fig. 2 we show the phase shifts corresponding to a single vacancy and a LV in the direction of the most stable edge dislocation in the lattice, namely the [110] direction. We note that as in the case of the isolated vacancy, the LV introduce a localized state in the dip of the density of states at $E=0.0$ (see Fig. 2), and that both phase shifts are strikingly similar. This similarity should be a consequence of the nondirectionality of the s states and does not hold for higher-energy regions, where a full sp^3 Hamiltonian is needed.[15,16] We note that the result shown in Fig. 2 cannot be compared with those obtained by other authors by means of much more elaborate calculations[15,16] because the changes in the lower part of the valence band were not discussed by the previously mentioned authors.

We return to the sc lattice and consider an aspect of our results more interesting than the phase shifts shown in Fig. 1. In Fig. 3 we show the formation energy of the three main LV in the sc lattice as a function of the position in the band of the Fermi level. This energy has been calculated by obtaining the difference in energy between N isolated vacancies or the same N vacancies forming a line. The result is strikingly similar to the interaction energy of two single vacancies (see Fig. 4 of this paper and Fig. 1 of Ref. 14); this is a consequence of the very weak interaction between second-nearest-neighbor vacancies along the three directions herewith considered (see Ref. 14). On the other hand, our result points in the same direction as the well-known fact concerning dislocations in the sc lattice, namely, that the most stable edge dislocation in this lattice has its line in the [100] direction.[21] In fact, our results (see Fig. 3) indicate that a vacancy line in the [100] direction is more stable, no matter how full the band, than in the other two directions. It must be noted that in absolute terms, no vacancy line should be stable, and if one is formed through, say, annihilation of two edge dislocations of opposite signs, it should decompose in voids of either spherical or disk shape.

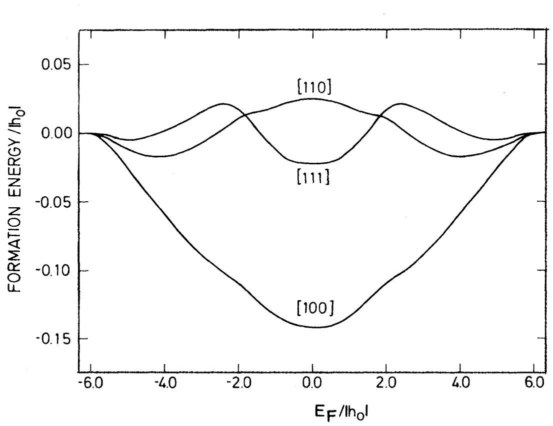

FIG. 3. Formation energy (see text) for LV in the main three directions of the sc lattice as a function of the position of the Fermi level. All energies are referred to the nearest-neighbor interaction h_0.

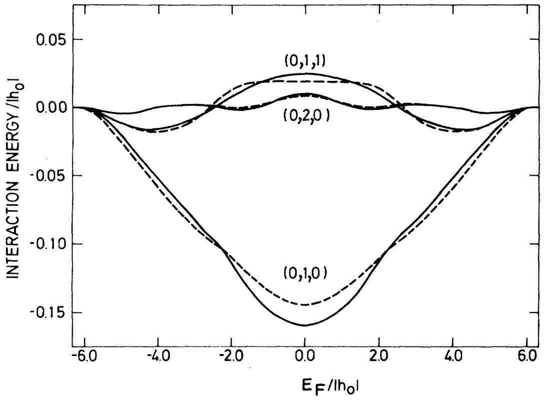

FIG. 4. Interaction energy between parallel LV being separated by lattice vectors (1,1,1), (0,2,0), and (0,1,0). The interaction energy between single vacancies separated by the same vectors is also shown (dashed lines).

Finally, we discuss our results for the interaction energy between LV in the same crystallographic direction. We concentrate on the most stable direction, namely, the [100] direction. In Fig. 4 we show our results for LV separated by three vectors, (0,1,1), (0,1,0), and (0,2,0). This figure also shows the results for the interaction between single vacancies. The most remarkable aspect of this study is that both the interaction between single vacancies and that between LV are very similar. Again this seems to be a consequence of the very low interaction between second-nearest-neighbor vacancies. Before ending this discussion we also note that the interaction between LV shows Friedel oscillations very similar to those shown by the interaction between single vacancies.[14] This result should be a consequence of the rather weak anisotropy of the sc lattice, which leads to a Fermi surface very close to a sphere. A complete discussion of this point can be found in Ref. 13.

IV. CONCLUDING REMARKS

In this paper, we have extended the scattering theoretical method, which is being widely used ot handle the problem of defects in solids as well as surfaces and interfaces,[1-14] to treat the more complex problem of line defects. We have shown that this method can solve very easily the case of LV, eliminating the need for superlattices. Although the method can also be used to treat any other line defect in which the breaking of the crystal symmetry is weak, such as lines of divacancies (this case has been solved in this paper when the interaction between LV was considered; see also Ref. (15) or sets of dislocations whose Burgers vectors add to zero (see the Appendix), it cannot be applied to the case of an isolated dislocation where a very severe breaking of crystal symmetry takes

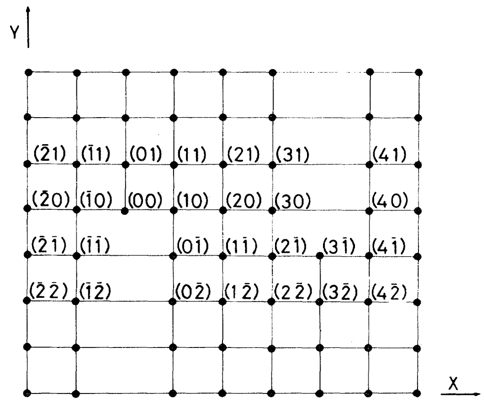

FIG. 5. Atomic positions of the atoms on the plane $z=0$ of a sc lattice with two edge dislocations parallel to the [001] direction and with opposite Burgers vectors. The problem-adapted numeration of the atomic positions is particularly important. The strength of all the bonds (solid lines) is h_0.

place[22] (see also Ref. 19).

We have applied the method to the simplest case, that of the sc lattice with a single orbital per atom. We have discussed the very strong similarities between the case of LV and that of isolated vacancies; this is a direct consequence of the nondirectionality of bonding associated with s electrons. Similar conclusions are found for the diamond lattice with a single s orbital per atom. The study of the formation energy of the LV has allowed us to conclude that the LV in the [100] direction is the most stable; this result is in agreement with the well-known fact that the most stable dislocation line in the sc lattice occurs in the [100] direction.

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APPENDIX: DISLOCATIONS IN THE sc LATTICE

As in Sec. III, the Hamiltonian involves one s state per site and interactions are restricted to nearest neighbors. The system that we study is shown in Fig. 5; it possesses two edge dislocations running along the [001] direction with opposite Burgers vectors, a (1,0,0) and a $(-1,0,0)$, respectively. The distance between the dislocations is $4a$.

We write the Hamiltonian of the perturbed system using the problem-adapted notation shown in Fig. 5. The difference between this Hamiltonian and the Hamiltonian of the perfect sc lattice is

$$V=h_0\sum_{m_3=-\infty}^{\infty}\big(-|00m_3\rangle\langle 0\bar{1}m_3|+|10m_3\rangle\langle 0\bar{1}m_3|-|10m_3\rangle\langle 1\bar{1}m_3|+|20m_3\rangle\langle 1\bar{1}m_3|-|20m_3\rangle\langle 2\bar{1}m_3|$$
$$+|30m_3\rangle\langle 2\bar{1}m_3|-|30m_3\rangle\langle 3\bar{1}m_3|+\mathrm{H.c.}\big)\,, \qquad \text{(A1)}$$

where only an infinite sum along the direction of the dislocation appears. Now, the direction of the dislocation is Fourier-transformed in the way explained in Sec. II. The Fredholm determinant [Eq. (5)] factorizes in the mixed representation (see Sec. II), remaining an effective 8×8 block for each wave vector k. The reduced dimension for each k is a result of the localized nature of the perturbation V [Eq. (A1)] in the position coordinates of the plane perpendicular to the dislocation. Finally, the phase shift is given by

$$\delta(E)=\sum_{k\in 1\mathrm{DBZ}}\arg D(E,k)\,, \qquad \text{(A2)}$$

where $D(E,k)$ stands for the 8×8 generic block of the Fredholm determinant.

The preceding analysis remains valid for more distant dislocations or for a set of dislocations with Burgers vectors adding to zero. The main difference is only the dimension of the pertinent block of the Fredholm determinant. It increases as the complication of the studied system grows.

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