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Green functions for superlattices

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A Green-function investigation is made of the (complex) band structure and local density of states of superlattices composed of two alternating component crystals, which are modeled by means of the two-band nearly-free-electron approximation. The variation of different superlattice band structures with component-crystal thickness is studied in detail, particular attention being paid to the all-important role played by interface states.

I. INTRODUCTION

The band structure of superlattices, especially those prepared by molecular-beam epitaxy (MBE), has been investigated intensively in recent years. The first simple models, with rectangular barriers,[1] have now been superseded by more sophisticated calculations, which can describe real systems.[2] These calculations are rather demanding numerically, so simplified formulations, particularly for thicker component crystals, have also been developed.[3]

Here, a straightforward Green-function (GF) approach is adopted, which provides a means of describing the electron energy bands and gaps of a superlattice in terms of the solutions of the Schrödinger equation, satisfying one-sided boundary conditions at infinity. A study is performed of the development of the band structure, i.e., the modification of the energy gaps of infinite crystals, and the formation of new gaps as the thickness of the component crystals is varied. Special attention is paid to the role of interface states, since superlattices may be viewed as systems with many interfaces.[4–6] Isolated interfaces between two crystals can either contain such localized states, or be free of them, so these properties can be expected to be reflected in the related superlattices. To illustrate the general properties, a simple one-dimensional model in the two-band nearly-free-electron (NFE) approximation is adopted, for which two types of interfaces are easily obtained by merely changing a single parameter in the effective potential.

II. FORMULATION

In atomic units ($\hbar = 2m = 1$), the GF $G(x,x';z)$ in the coordinate representation is given by

$$[z+\nabla_x^2 - V(x)]G(x,x';z) = \delta(x-x') \ , \tag{1}$$

where $z = E + i0$. Although there are several ways to construct the GF, the so-called direct method[7,8] is used here, where the GF is expressed in terms of the solutions of the corresponding Schrödinger equation, satisfying one-sided boundary conditions. For infinite systems,

$$G(x,x';E) = \frac{f_+(x)f_-(x')\Theta(x-x') + f_-(x)f_+(x')\Theta(x'-x)}{W[f_-,f_+]} \ , \tag{2}$$

where f_+ and f_- are the solutions of the Schrödinger equation for energy E, satisfying the physical boundary conditions at $+\infty$ and $-\infty$ (i.e., outgoing propagation of electrons in the bands, and decaying solutions in the gaps). In the denominator, the Wronskian of f_+ and f_- is independent of x. The poles of the GF determine the energies of the discrete eigenstates, and the local density of states (LDOS) at x is given by

$$D(x;E) = -\pi^{-1}\,\mathrm{Im}\,G(x,x;E+i0) \ . \tag{3}$$

The superlattice to be investigated consists of alternating layers of A and B crystals, the potential $V(x)$ being equal to that of crystal A (B) over the domain of length d_A (d_B). The infinite system is periodic, with a period $d = d_A + d_B$, so solutions of the Schrödinger equation will have a Bloch form with real wave numbers k from the Brillouin zone $-\pi/d \le k \le \pi/d$, and the dispersion relation $E(k)$ will exhibit allowed and forbidden energy bands (the latter corresponding to complex wave numbers). In the allowed bands, the group velocity $\nabla_k E_n(k)$ of an electron enables the correct assignment of f_+ and f_- to the Bloch functions to be made.

Since the systems to be modeled are prepared by MBE, the interatomic distances in the two crystals forming the superlattice have to be very close. Therefore, model potentials with the same periodicity a are used for both crystals A and B. As the aim is to understand general trends, rather than to describe actual structures, the simple NFE approximation is employed for the two crystals. The potential in the first unit cell is then

$$V(x) = \begin{cases} V_A + W_A\cos(gx), & -N_A a/2 \le x \le N_A a/2 \\ V_B + W_B\cos(gx), & N_A a/2 \le x \le (N_A/2 + N_B)a \end{cases} \tag{4}$$

where $g = 2\pi/a$, N_A (N_B) is the number of atoms in the crystal A (B), and d_A ($= N_A a$) is kept equal to d_B ($= N_B a$).

The solutions f_+ and f_- are now obtained for the system, using (4), by the following procedure. Inside any domain A or B for each energy, two independent solutions of the Schrödinger equation can be found from the solution for the infinite NFE crystal, satisfying one-sided boundary conditions,[9] namely

$$\phi_{\pm}(x) = \exp[\pm i(\xi^2 - V^2)^{1/2} x/g]\{\exp(igx/2) + V^{-1}[\xi \mp (\xi^2 - V)^{1/2}]\exp(-igx/2)\}\ , \tag{5}$$

where $\xi = z - V - g^2/4$. The complete solution is obtained by quantum mechanically matching these domain solutions at the interfaces. Because of the periodicity of the superlattice, only two matchings between A and B crystals are needed, complemented by the Bloch theorem requirement.

Using the inversion symmetry of the potentials, a linear combination of the functions (5) in A can be formed, in such a way, that at the origin one of the solutions is of unit value and zero slope, while the other is of zero value and unit slope. This simplifies the evaluation of the Wronskian in (2) (such even and odd solutions have also been used for piecewise constant potentials[10]). These solutions are then matched at $x = N_A a/2$ with the solutions in B. After the next matching at $x = (N_A/2 + N_B)a$, the two solutions at $d = (N_A + N_B)a$ can be evaluated. The final solutions for the superlattice, which satisfy the requirements of Bloch's theorem, can then be formed by proper linear combinations of the two solutions: $f_k(d) = e^{ikd} f_k(0)$. From the boundary conditions, for each energy E, the pair $f_{k+}(x)$ and $f_{k-}(x)$, needed in (2), results.

III. ELECTRONIC PROPERTIES OF SUPERLATTICES

The one-band approximation[11] can be used to describe superlattices formed from two kinds of crystals whose valence and conduction-band edges are only slightly different. However, it has been shown[12] that this approximation fails, even qualitatively, when for example the top of the valence band of one of the component crystals lies close to the bottom of the conduction band of the other. In such a case, the two-band description of the crystals is required. The band structure of such superlattices has been investigated.[12] For very thin films, dispersion relations $E(k)$ have been obtained and compared with the results of the one-band approximation, and, for thicker films, the thickness dependence of the gap has been given. The analysis showed that, by varying the thickness of the two component crystals, a material can be obtained whose band structure bears little resemblance to that of either of the component crystals. Indeed, the new properties seemed to be governed by the relative positions of the band edges.

The analysis of a superlattice—viewed as a system with many interfaces between the crystalline components[4–6]—can be started from that of a single interface. As far as the band structure of two ideal crystals in contact is concerned, two classes can be distinguished: systems with interface states, localized only in the vicinity of the interface, and those without any such states. If the number of interfaces is increased to form a superlattice, the two classes should exhibit different behaviors, because the interaction between the former interfaces should induce the formation of an interface band from the isolated interface state. The relative importance of this band is expected to increase, as the thickness of the component crystals decreases, thus giving rise to qualitatively different band structures in the two cases. Although interface states on isolated interfaces differ in their space localization from the remaining delocalized states, this distinction tends to disappear on forming the superlattice, resulting in a kind of hybridized behavior. Consequently, not only the band structure of the two crystals, but also their coupling at the interface, is expected to be an important factor in determining the band structure of the composite system.

In the NFE approximation of the two crystals, the gap widths are determined by the magnitude of the Fourier components of the potentials, whereas the coupling depends on the relative phases of the components as well. The simplest case of an interface between two NFE crystals is that where the crystals have equal gaps at the same energies. The magnitudes of the two potentials are then the same and, in order to distinguish different couplings, the cases when the two Fourier components are (a) identical and (b) of different sign will be discussed. Here, only superlattices with crystals of equal thickness ($d_A = d_B = d/2$) are considered.

In the first case (with no interface state), the system's periodicity is a, and a simple band structure of an infinite NFE crystal is obtained, without any dependence on d.

The band structure for the model which has an interface state in the middle of the gap is shown in Fig. 1(a). The interface band broadens as d decreases, filling the gap of the infinite crystal at $d \approx 60a$. This behavior corresponds to earlier findings, where the interaction between two states, localized on opposite sides of a thin film, have been studied.[9,13] In Fig. 1(c) is displayed the complex band structure of the system with $d = 80a$. The interface band, centered at $E = 1$, is separated from the other branches of the band structure by gaps bridged by complex loops. These gaps arise as a consequence of the increased period of the system, which is accompanied by the cutting of the original Brillouin zone into smaller segments. Note that, although the positions of the gaps are the same in the two cases discussed, the band structure around $E = 1$ is qualitatively different. Figure 1(b) depicts the LDOS curves corresponding to the interface-band case. The spatial distribution is given for the interface band ($E = 0.99$ and 1.00) and for the next bands ($E = 0.96$ and 1.04). In the former case, an enhanced localization of the electrons at the interfaces is apparent. In contrast, in the two adjacent bands, the LDOS maximum is in the middle of the component crystal.

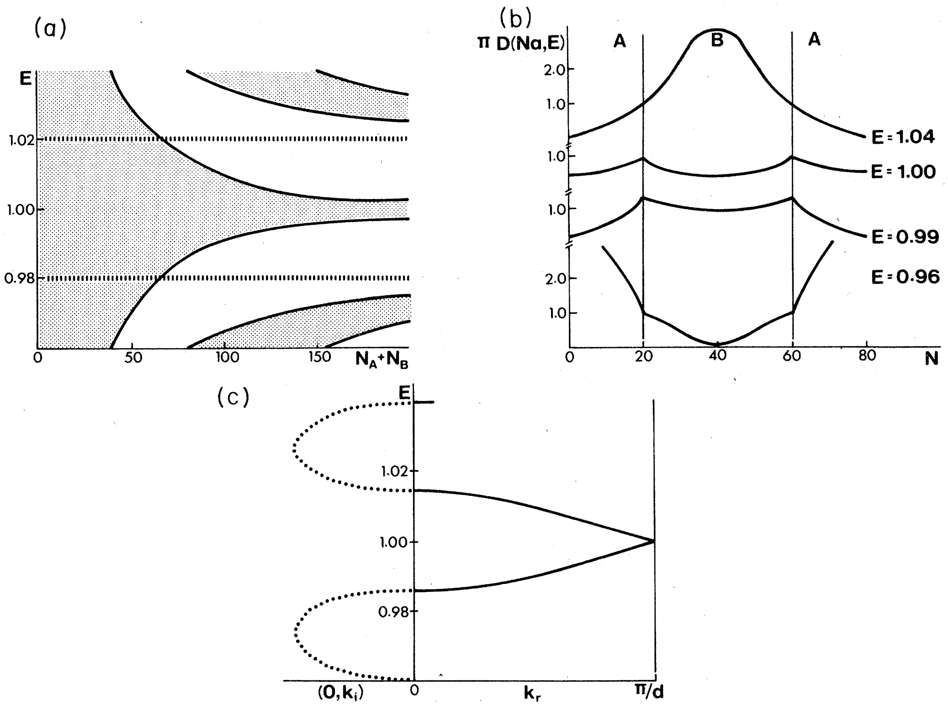

FIG. 1. Band structure of a superlattice with equal centered gaps. Potential $V(x)$ is given by (4) with $N_A = N_B$, $a = \pi$, $V_A = V_B = 0$, $W_A = -0.02$, and $W_B = 0.02$ (a.u.). (a) Energy bands (shaded areas) as functions of component thickness. Dashed lines depict the gap of the infinite crystals A and B. (b) Local density of states $D(x;E)$, where $x = Na$ (N being an integer), for a system with $N_A = N_B = 40$ in the interface band ($E = 0.99$ and 1.00) and in the two adjacent bands ($E = 0.96$ and 1.04). (c) Complex band structure at $N_A = N_B = 40$ with complex loops (dotted) connecting the real branches.

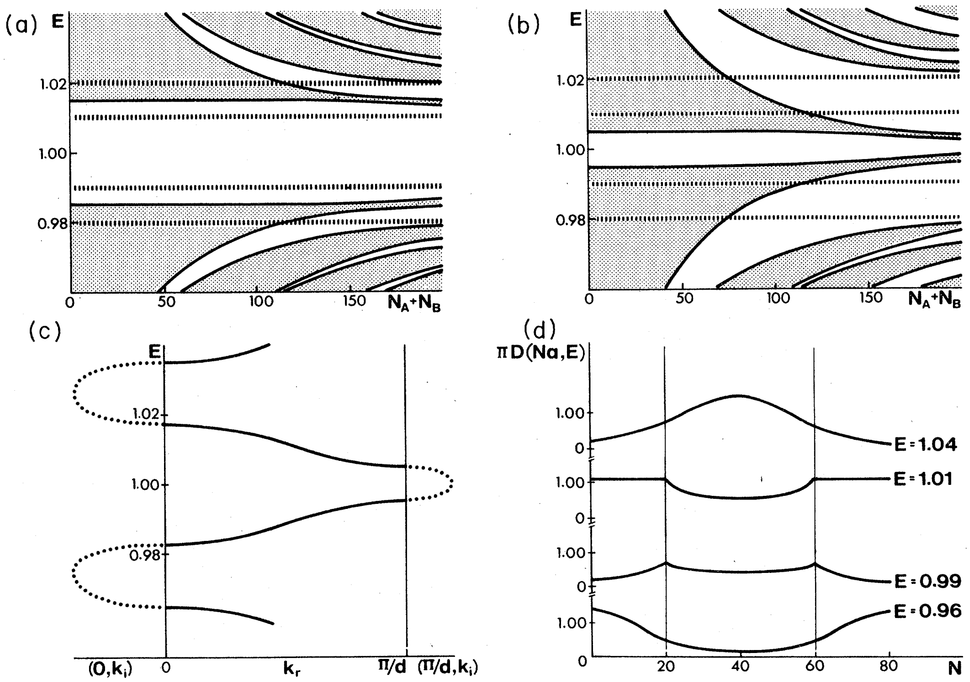

FIG. 2. Band structure of a superlattice with overlapping centered gaps. Potential (4) with $N_A = N_B$, $a = \pi$, $V_A = V_B = 0$, $|W_A| = 0.01$, and $W_B = 0.02$. Energy bands for a system: (a) without ($W_A = 0.01$) and (b) with ($W_A = -0.01$) an interface state at an isolated interface. (c) Complex band structure for (b) at $N_A = N_B = 40$. (d) Local density of states $D(x;E)$ for a system with $N_A = N_B = 40$ in the interface band ($E = 0.99$ and 1.01) and in the two adjacent bands ($E = 0.96$ and 1.04).

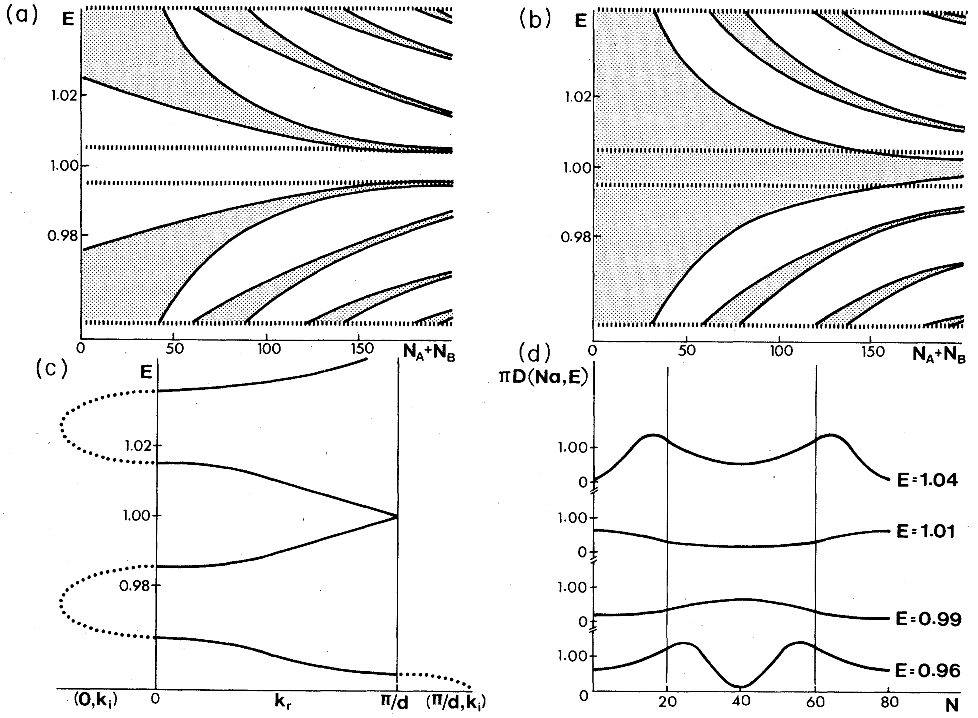

FIG. 3. Band structure of a superlattice with disjoint gaps. Potential (4) with $N_A=N_B$, $a=\pi$, $V_A=-0.025$, $V_B=0.025$, $|W_A|=0.02$, and $W_B=0.02$. Energy bands for a system (a) without ($W_A=0.02$) and (b) with ($W_A=-0.02$) an interface state at an isolated interface. (c) Complex band structure for (b) at $N_A=N_B=40$. (d) Local density of states $D(x;E)$ for a system with $N_A=N_B=40$.

If crystals with different gap widths, centered at $E=1$, are in contact, a rather different band structure is encountered around $E=1$. Figure 2 illustrates the d dependence of a superlattice formed by two NFE crystals with $|V_g|=0.01$ and 0.02. When the Fourier components are of equal or opposite sign, there is a gap around $E=1$, in each case. The gap is wider for the case of equal signs [Fig. 2(a)], where it remains constant and equal to the average value of the gaps of the two infinite crystals till about $100a$, after which it slowly narrows as d increases. For potential amplitudes of opposite sign (when, for a single interface, there is an interface state in the middle of the gap), as shown in Fig. 2(b), the gap is smaller, even than the gap of either infinite crystal, and is again constant till $\approx 100a$, when it gradually decreases with increasing d. As can be seen, in Figs. 2(a) and 2(b), other bands and gaps accumulate above and below the center gap. The complex band structure, corresponding to Fig. 2(b) at $d=80a$, is given in Fig. 2(c), and the LDOS in Fig. 2(d).

Finally, the case of two nonoverlapping gaps was investigated, and the results are presented in Fig. 3. The two crystals of the superlattice were chosen to have equal gaps ($|V_a|=0.02$) separated in energy by 0.05 (one having its center raised by 0.025 above $E=1$, and the other its center lowered by the same amount). The results for Fourier components with equal (opposite) signs are shown in Fig. 3(a)[3(b)]. Qualitatively different band structures are obtained around $E=1$ for the two cases. In Fig. 3(a), there is a gap in the middle (even though both infinite crystals have allowed bands in this region), while in Fig. 3(b) there is a band around $E=1$. The complex band structure for the case with opposite signs of the Fourier components at $d=80a$ is drawn in Fig. 3(c), and the corresponding LDOS curves are in Fig. 3(d).

IV. CONCLUSION

A simple method of constructing GF for superlattices in terms of the solutions of the Schrödinger equation for infinite crystals, satisfying one-sided boundary conditions, has been developed. Although the procedure was applied to one-dimensional systems with two alternating components, it can be extended in a straightforward manner to systems with more components, and also to three-dimensional problems.[14] If the GF is used in the context of the surface GF formalism, then finite superlattices can also be treated.

From a two-band model, based on the NFE description of its components, the trends in the variation of the band structure of a superlattice as a function of component thickness have been presented. For the cases of overlapping and disjoint gaps, the complex energy band structure and LDOS have been calculated. In particular, a qualitatively different behavior has been found for the two model cases differing only by the existence, or nonexistence, of localized interface states at their isolated interface. These findings indicate that the relative positions and magnitudes of the gaps are not sufficient by themselves to determine the properties of corresponding superlattices.

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