dent parts of $J(J_b, J_e, J_d)$ are of the orders $\alpha\beta^4\omega_0$ and $\alpha\beta^3\omega_0$, we can use in conjunction with them the zero-order approximation for F_g which reduces simply to a sum over unperturbed zero-phonon one-particle states.

[10]The δ-function potential is weak, because it is smeared over a region of the dimensions of the radius of the polaron $\rho_{e,h}$. Its strength is measured by the dimensionless quantity $\alpha_{e,h}e^2/(\hbar\omega_0\epsilon_s\rho_{e,h}) \approx \alpha\beta \ll 1$. Therefore, it can be treated as a perturbation.

[11]J. P. Walter and M. L. Cohen, Phys. Rev. B 2, 1821 (1970).

[12]S. D. Mahanti and C. M. Varma, Phys. Rev. Letters 25, 1115 (1970); and unpublished. Equation (10) of the letter contains a misprint: Its part printed as $(2\mu^{**}\omega_0)^{1/2}$ should read $(2\mu^{**}\omega_0)^{-1/2}$.

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Resonant Interactions between Localized LO Phonons and Continuum States of Donors in CdS and CdSe

C. H. Henry
Bell Telephone Laboratories, Murray Hill, New Jersey 07974

and

J. J. Hopfield*†
Department of Physics, Princeton University, Princeton, New Jersey 08540

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The first longitudinal-optical- (LO-) phonon replica of the I_2 line (decay of an exciton bound to a neutral donor) in CdS and CdSe is structured and broadened. The replica is roughly Lorentzian in shape, shifted to lower energy than the nominal LO-phonon energy and has a sharp notch near the center of the line. These features are shown to arise from coupling between LO phonons and the donor electron. The line is lifetime broadened by ionization of the donor. Virtual excitations of the donor result in frequency shifts and cross coupling of different LO-phonon modes. The notch is an interference effect resulting from the coupling of the localized mode existing immediately after the electron and hole recombine with less-damped modes, located more distant from the donor.

I. INTRODUCTION

In the last few years, longitudinal-optical-(LO-) phonon sidebands in the spectra of excitons, donors, and acceptors have received much attention. It has been established that LO-phonon modes of the perfect crystal are greatly modified by the electron-phonon interaction. The first studies were of excitons where Toyozawa and Hermanson[1] showed that the electron-phonon interaction leads to an attractive interaction which lowers the energy of the LO-phonon sideband of the exciton (observed in absorption). They predicted that in some circumstances (not observed experimentally) a bound state consisting of an exciton–LO-phonon complex could occur. In a second paper, Toyozawa[2] concluded that the observed exciton–LO-phonon sideband results from a quasibound state in which the LO-phonon–exciton complex immediately decays after formation into continuum states of the free exciton. Bound states, analogous to those predicted for excitons by Toyozawa and Hermanson, were found by Dean, Manchon, and Hopfield[3] for donors in GaP. These states consist of s- and p-like LO-phonon local modes bound to the neutral donors. The authors observed these modes by Raman scattering and by luminescence. These modes were also observed by Barker[4] using infrared absorption. Similar LO-phonon local modes associated with acceptors in CdS.

In the case of donors in GaP and acceptors in CdS, the LO-phonon energy is less than the energy of the first excited state of the bound electron (or hole). In this case, the interaction is attractive and a local mode is readily formed.[3] The situation is quite different for donors in direct band-gap semiconductors. In almost all cases the LO-phonon energy $\hbar\omega_0$ is greater than the donor binding energy E_D. This situation is depicted by the energy diagram in Fig. 1. A bound state cannot exist, because such a state would be degenerate with the free-electron continuum of the donor and will spontaneously decay by ionization of the donor. Instead we expect the state will be quasibound in analogy with the exciton case previously discussed by Toyozawa.[2]

In this paper we report the observations of LO-phonon sidebands in the decay of excitons bound to neutral donors in CdS and CdSe. The sidebands are shifted to a lower phonon energy than the LO phonon in the perfect crystal and broadened, as qualitatively predicted by Toyozawa.[2] Besides

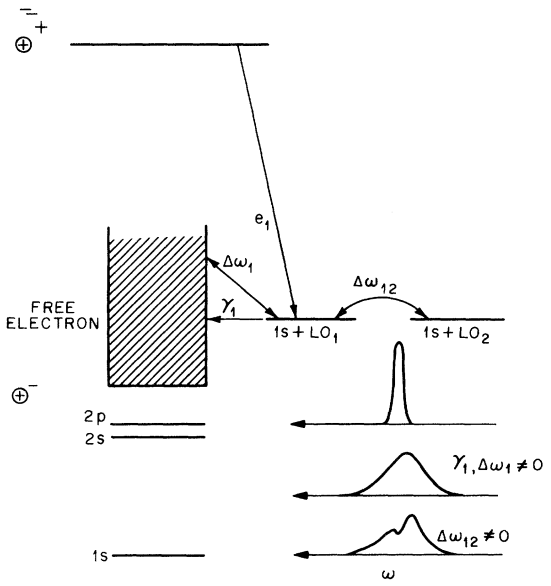

FIG. 1. Energy-level diagram indicating the initial state of the bound exciton and the final states. The final states include the bound electron and continuum states of the donor with no LO phonons excited and one-LO-phonon modes with the electron in the 1s state. The diagram also indicates how the LO-phonon line shape changes as a result of ionization of the donor and virtual excitations of the donor which result in frequency shifts and cross coupling of the LO-phonon modes.

these features, the sidebands are structured having a notch near the center of the broadened line. This interference effect has not been theoretically anticipated.

Reynolds, Litton, Collins, and Frank[6] observed broadening and structure in the LO-phonon replica of the I_2 line (exciton bound to a neutral donor) in CdS and ZnO. They interpreted the structure as due to the anisotropy of the LO phonons in these crystals. We have not considered the case of ZnO. For the case of CdS, the effect of anisotropy can be observed in the broadening of the LO-phonon replica of the I_1 line (decay of an exciton bound to a neutral acceptor) and in Raman scattering. But this broadening accounts for only one-fourth of the width of the I_2 line and it also does not account for the observed structure. We will neglect this source of broadening.

We will show that the broadening, line shifts, and the notch in the line are all consequences of the electron-phonon coupling. The observed line shapes are discussed in Sec. II. In Sec. III the physics of the line shape is discussed, a formal theory of the line shape is derived, and finally an approximate solution is obtained, which adequately represents the experimental data.

II. OBSERVATIONS

The solid curve in Fig. 2 is a photomultiplier recording of the LO-phonon replica of the I_2 line in CdS. Similar line shapes were observed for LO-phonon replicas of the I_2 lines associated with six different donors. The width and position of the isolated LO phonons (those far from the donor) are also shown in Fig. 2. The same width and position of the isolated LO phonons was observed both by Raman scattering and by measurements of LO-phonon replicas of the I_1 line. The figure shows that the peak of the LO-phonon replica of the I_2 line is shifted to lower phonon energy by ≈ 1 meV, that the line is Lorentzian in shape with a full width of ≈ 1.6 meV, and that a dip occurs in the high-energy side of the peak but lower in energy than the isolated LO-phonon energy.

A similar spectrum was observed for the LO-phonon replica of the I_2 line in CdSe. The line shape was recorded photographically and is not as accurate as the photomultiplier recording for CdS. The phonon replicas of the I_1 and I_2 lines in CdSe are shown in Fig. 3. The LO-phonon replica of the I_1 line is only 0.25 meV wide, whereas the LO-phonon replica of the I_2 line is 1.1 meV wide. Just as in the case of CdS, there is a notch in the broadened line, occurring slightly to the high-energy side. If we interpret the energy and width of the LO-phonon replica of the I_1 line to represent the isolated LO phonons, then the center of the line shape as well as the notch are at lower energies than the isolated LO phonons. We do not have as much data for CdSe as we do for CdS, but we have observed the same I_2-line LO-phonon replica in two samples from different crystal growths.

The methods of sample preparation and other features of the spectra have been previously reported by Henry, Nassau, and Shiever.[7-9]

III. THEORY

A. Physical Interpretation

Because the general theory of the line shape to be expected in this particular bound-exciton annihilation process is so complex, we will begin by attempting to isolate the qualitative factors which must be responsible for the observed line shape. All unessential theoretical elements will be discarded, and more quantitative theoretical considerations will be made only for the simplified model.

Because of thermalization in the initial state, the lowest-energy state of an exciton bound to a neutral donor is the unique initial state for the process under study. The possible electronic and vibrational final states and emission processes

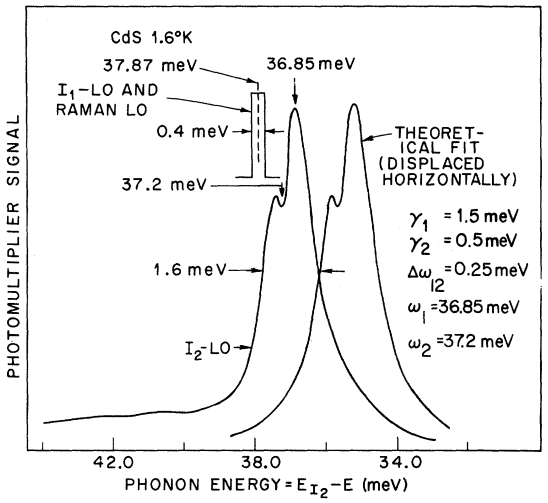

FIG. 2. Solid line shows the LO-phonon replica of the I_2 line in CdS. The insert shows the energy and width of the nominal LO phonons in CdS. The dashed curve is the theoretical curve, Eq. (13), using the parameters indicated in the figure.

are shown schematically in Fig. 1. At the interesting energy I_2-LO, only two final states are important, the final state in which the donor is in its ground (1s) state and an optical phonon is created, and the final state in which the donor is ionized. Each of these in itself represents many states, for there are many wave functions possible for the final-state phonon or the final-state free electron.

The general shape of the observed spectrum suggests an interference effect, the most obvious of which would be the interference between the $1s$ + LO state and the continuum on which it lies. The shape of such an effect would, however, yield a Breit-Wigner form, quite unlike the observed shape. (In addition, the continuum on which the observed line sits is negligibly weak, and direct coupling to the continuum can be neglected.)

The observed line shape appears like an interference between two states, *both located very near the nomial* LO *frequency*, one of them sharp (causing the sharp notch) and the other broader (giving the over-all ~1.6-meV width to the spectrum in CdS). The physical origin of such states can be found in the localizability of optical phonons. If dispersion in the LO branch is neglected, localized optical phonons can be chosen as a basis, and will all have the same frequency and the same small damping in a perfect crystal. In the presence of a donor, the local optical phonons located near the donor will interact with the donor electron. These modes will be damped through the process: local optical phonon + neutral donor → ionized donor + free electron. This step, used as a virtual process, will also produce frequency shifts of the local modes, and will couple modes located in one place with spatially nearby modes. Optical phonons at different distances from the impurity thus represent the interfering species. The modes near the donor are broad, while the distant modes are narrow and provide the origin of a sharp interference effect and the narrow notch in the spectrum. The method of damping and cross coupling is the excitation of the neutral donor. While the dispersion of the optical-phonon branch will slightly alter the argument, dispersion effects are small for the long-wavelength phonons of relevance to the centers under discussion.

B. Mathematics of Line Shape of LO-Phonon Replica

The transition rate for the decay of a bound exciton emitting a photon of energy $\hbar\omega$ is given by the "golden rule"

$$w(\hbar\omega) = (2\pi/\hbar)\sum_f |\langle f|H_{\rm rad}|i\rangle|^2 \delta(E_i - E_f - \hbar\omega) , \quad (1)$$

where i and f represent initial and final vibronic states, $H_{\rm rad}$ is the coupling to the electromagnetic field, and E_i and E_f are the initial- and final-state energies. To simplify the calculation (but lose no known essential part) we presume the initial wave function can be adequately represented by a product function,

$$|i\rangle \sim v(\vec{r}_{e_1})\uparrow v(\vec{r}_{e_2})\downarrow w(\vec{r}_h)\chi , \quad (2)$$

a product of the wave function of the first electron, the second electron, the hole, and the lattice wave function χ. The two electron spins are denoted by arrows. The radiative transition annihilates one electron and the hole, leaving the other electron in state $v(\vec{r}_e)$ and the lattice in state

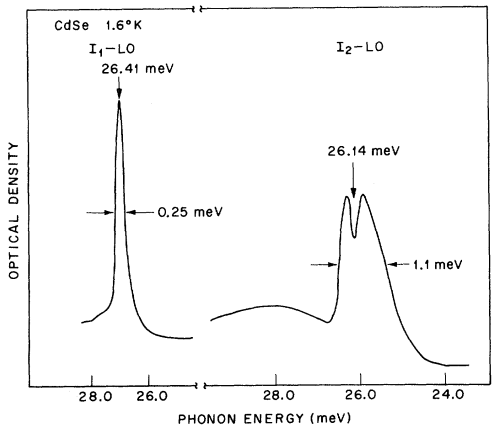

FIG. 3. LO-phonon replicas of the I_1 and I_2 lines in CdSe. The I_1-line replica is a good measure of the width and position of the nominal LO phonons in CdSe. The data were taken photographically.

χ. The normalized line shape $I(\omega)$, suppressing all factors of $\hbar$, is then

$$I(\omega)=\sum_f |\langle f|\, v(\vec{r}_e)\,\chi\rangle|^2 \delta(E_i - E_f - \omega)\ . \tag{3}$$

If we measure frequency in terms of ω', the frequency shift below the I_2 line, defined by

$$\omega \equiv E_i - E_{1s} - \omega'\ , \tag{4}$$

and substitute the Fourier transform of the δ function in Eq. (3), we have

$$I(\omega') = (1/2\pi)\sum_f |\langle f|\, v(\vec{r}_e)\,\chi\rangle|^2 \int_{-\infty}^{\infty} e^{i(\omega' - E_f + E_{1s})t}\, dt$$

$$= (1/2\pi)\int_{-\infty}^{\infty} e^{i\omega' t}\langle v(\vec{r}_e)\,\chi|\, e^{-iH't}\, v(\vec{r}_e)\,\chi\rangle\, dt\ , \tag{5}$$

where

$$H' \equiv H - E_{1s}\ .$$

Equation (5) can be written as a sum of two integrals with limits from zero to infinity which can be combined as

$$I(\omega') = (1/\pi)\,\mathrm{Re}\int_0^{\infty} e^{i\omega' t}\langle v(\vec{r}_e)\,\chi|\, e^{-iH't}\, v(\vec{r}_e)\,\chi\rangle\, dt\ . \tag{6}$$

The only significant approximation so far present is the use of a product wave function, without which the state in (6) would represent a correlated vibronic wave function rather than an uncorrelated one.

The line-shape calculation has been reduced to finding the time evolution of a single state containing one electron (in the state it would have immediately after annihilation of the hole with the other electron) and the lattice. Consider first the electronic part of this state. If there were no electron-phonon coupling, the spectrum would be determined by the electronic state alone, which would be a linear combination of $1s$, $2s$, ... and continuum electronic states with amplitudes a_{1s}, a_{2s}, ... The observed spectrum would then be

$$|a_{1s}|^2 \delta(E_i - E_{1s} - \omega) + |a_{2s}|^2 \delta(E_i - E_{2s} - \omega)\cdots\ .$$

The fact that two-electron transitions (i.e., those in which the final-state electron is not in the $1s$ state) are weak, and the two-electron continuum is very small compared to the emission of interest, allows one to assume $a_{2s}=0, \ldots,$ and thus that

$$v(\vec{r}) \approx \psi_{1s}(r)\ .$$

The phonon wave function should best be written in terms of the lattice equilibrium, with the donor in the $1s$ state. In terms of this state, the state χ contains zero-phonon, one-phonon, two-phonon, etc. parts. The zero-phonon part simply gives rise to the ordinary zero-phonon I_2 transition. The one-phonon part of the state causes those transitions which occur near $I_2 - \mathrm{LO}$ and are thus interesting, while the two-phonon part generates optical transitions at lower energies and will be ignored. For weak perturbations (and the strength of $I_2 - \mathrm{LO}$ is small compared to I_2), the amplitude of the initial one-phonon state can be described as a linear combination of phonons $|k\rangle$ with amplitudes b_k^0, and that *part* of the initial vibronic wave function which involves one phonon is thus

$$v(\vec{r})\,\chi_1 \equiv \sum_k \psi_{1s}(r)\, b_k^0 |\, k\rangle\ .$$

The spectral shape $I_1(\omega)$ of the one-phonon region of the spectrum is found by substituting this wave function into (6). If the amplitude of the one-phonon no-electronic-excitation state is described by $b_k(t)$ and if we take the initial conditions to be

$$b_k(0) = b_k^0\ ,\quad b_k(t) = 0\ ,\quad t<0 \tag{7}$$

the shape of the one-phonon line is given by its transform $b_k(\omega')$:

$$I_1(\omega') = (1/\pi)\sum_k \mathrm{Re}[b_k^{0*}\, b_k(\omega')]\ . \tag{8}$$

Equation (8) is the starting point for the calculation of the experimentally interesting line shape $I_1(\omega')$ of the one-optical-phonon sideband of the I_2 transition.

The equations of motion of b_k involve the states to which the phonons are coupled, namely, states in which no phonons are present, but the electron has been excited into an excited state (normally a continuum state) $\psi_l(\vec{r})$. Let the amplitude for such a wave function be a_l. The equations of motion of the coupled amplitudes a_l and b_k are

$$i\dot{a}_l = (E_l - E_{1s})\, a_l + \sum_{k'} H'_{lk'}\, b_{k'}\ , \tag{9a}$$

$$i\dot{b}_k = \omega_0\, b_k + \sum_l H'_{kl}\, a_l\ . \tag{9b}$$

The collection of states being handled has been restricted to those of Fig. 1 in the vicinity of the $1s$ $+\hbar\omega_0$ energy. The matrix element $H'_{k'l}$ is that of the electron-phonon interaction, and for optical-mode phonons it is

$$H'_{kl} = \left(\frac{2\pi e^2}{V\hbar\omega_0}\right)^{1/2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)^{1/2} \times \frac{1}{ik}\int \psi_{1s}(r)\, e^{i\vec{k}\cdot\vec{r}}\, \psi_l^*(r)\, d^3r\ .$$

These equations can be solved, subject to the desired initial conditions, by adding $ib_k^0\,\delta(t)$ to the right-hand side of Eq. (9b)[10]:

$$\omega a_l(\omega') = (E_l - E_{1s})\, a_l(\omega') + \sum_{k'} H'_{kl'}\, b_{k'}\ ,$$
$$\omega b_k(\omega') = \omega_0 b_k(\omega') + ib_k^0 + \sum_{l'} H'_{kl'}\, a_{l'}(\omega')\ . \tag{10}$$

To avoid singularities, we may include a small damping of the a_l states,

$$E_l \to E_l - i\epsilon ,$$

and then eliminate the terms a_l in Eq. (10):

$$(\omega_0 - \omega')\, b_k(\omega') - \sum_{k'} \sum_{l} \frac{H'_{kl} H'_{lk'}\, b_{k'}(\omega')}{E_l - E_{1s} - \omega' - i\epsilon} = -ib_k^0 . \tag{11}$$

Equation (8) and (11) completely determine the line shape.

C. Two-Mode Model

The coupled equations, Eq. (11), cannot be solved exactly. The problem is to try to see how these equations represent the physics described in Sec. III A. The amplitude of the initial optical-mode lattice distortion falls off rapidly with distance from the donor, for it is driven by the electric field of the electron and hole which recombine. Outside the center, there is no field from this pair since the pair as a whole is neutral. The initial lattice distortion thus lies within the electron-hole-pair cloud. This distortion is approximately a normal mode, and is strongly damped by processes in which the 1s donor electron is ionized. It is the first mode of a two-mode model.

There are modes further away from the donor which are only weakly damped, and are also weakly coupled through virtual excitation of electron-hole pairs to the first mode. Since all these weakly damped modes have essentially the same frequency, they can be combined into a second mode, sharp compared to the first but weakly coupled to it. In this case, the line-shape problem can be solved exactly. Equation (11) reduces to

$$\begin{aligned} &(\omega_0 - \omega' - \Delta\omega_1 - \tfrac{1}{2}i\gamma_1)\, b_1(\omega') \\ &\qquad + (\Delta\omega_{12} + \tfrac{1}{2}i\gamma_{12})\, b_2(\omega') = -ib_1^0 , \\ &(\Delta\omega_{21} + \tfrac{1}{2}i\gamma_{21})\, b_1(\omega') + (\omega_0 - \omega' - \Delta\omega_2 - \tfrac{1}{2}i\gamma_2)\, b_2(\omega') = 0 . \end{aligned} \tag{12}$$

In this equation the expected form of line-shift parameters has been inserted as well as the linewidth parameters. The effect of the coupling term γ_{12} is to cause a small additional broadening of the line. We will neglect this term and take $\Delta\omega_{21} = \Delta\omega_{12}$. Then, if we define the mode frequencies

$$\omega_1 \equiv \omega_0 - \Delta\omega_1 , \quad \omega_2 \equiv \omega_0 - \Delta\omega_2 ,$$

$I_1(\omega')$ is given by

$$I_1(\omega') = \frac{\mathrm{Re}}{\pi} \left[-i \left| b_1^0 \right|^2 \Big/ \left(\omega_1 - \omega' - \tfrac{1}{2}i\gamma_1 - \frac{(\Delta\omega_{12})^2 (\omega_2 - \omega' + \tfrac{1}{2}i\gamma_2)}{(\omega_2 - \omega')^2 + (\tfrac{1}{2}\gamma_2)^2} \right) \right] . \tag{13}$$

Away from the ω_2 resonance,

$$I_1(\omega') \approx \left| b_1^0 \right|^2 \frac{\gamma_1/2\pi}{(\omega_1 - \omega')^2 + (\tfrac{1}{2}\gamma_1)^2} ,$$

giving the observed Lorentzian shape. Near the ω_2 resonance,

$$I_1(\omega') \approx 2 \left| b_1^0 \right|^2 \Big/ \pi\gamma_1 \left(1 + \frac{\gamma_2}{\gamma_1} \frac{(\Delta\omega_{12})^2}{(\omega_2 - \omega')^2 + (\tfrac{1}{2}\gamma_2)^2} \right) ,$$

resulting in a narrow notch near ω_2.

The experimental line shape for CdS is shown in Fig. 2. An exellent fit to this data, based on Eq. (13), is also shown in this figure. The parameters for the theoretical curve were determined in the following way. ω_1 and ω_2 were chosen to fit the energies of the peak and the notch, γ_1 was chosen to fit the linewidth, γ_2 was chosen to fit the width of the notch, and then $\Delta\omega_{12}$ was chosen to fit the magnitude of the notch. The values of these parameters are shown in the figure.

The LO phonons of the pure crystal have an energy of 37.87 meV and a linewidth of 0.4 meV, due mainly to the anisotropy of the LO-phonon frequency. LO-phonon modes very distant from the donor must also have these features. Modes 1 and 2 are altered from the distant LO-phonon mode as follows. Mode 1, representing the initial lattice distortion, is lowered in energy by about 1 meV. It is broadened by damping to a linewidth of 1.5 meV and, unlike the distant LO phonons, it is Lorentzian in shape. Mode 2, representing less-damped modes further away from the donor but coupling significantly and producing the notch, is lowered in energy by about 0.7 meV. The best fit to the experimental data gave a linewidth of this mode of 0.5 meV, slightly greater than that of the distant LO phonons, although this parameter could not be accurately determined.

No attempt was made to fit the data in CdSe, where the line shape (obtained from a densitometer trace of a photographic plate) was less accurately known.

IV. SUMMARY

The line shapes of the I_2-line LO-phonon replica in CdS and CdSe are structured and broadened. In both crystals the line is broader and lower in phonon energy than the nominal LO phonons. The line is also structured by a sharp notch near its center. In contrast to this, the I_1-line LO-phonon replica in CdS and CdSe is narrow and not shifted in energy. All of these features are consistent with coupling between the LO phonons and the donor electron. The line is broadened by ionization of the donor electron. Virtual excitations of the donor electron result in frequency shifts and cross couplings of the LO-phonon modes.

A formal theory of the line shape was derived. It involved an infinite set of coupled oscillator equations. This was then approximated by two coupled oscillators, one representing the initial LO-phonon mode existing immediately after the

electron and hole recombine and the other representing the less-damped more distant LO-phonon modes. In this model, the sharp notch arises from an interference caused by coupling the two oscillators. The theoretical line shape based on this model fitted the data very well. However, we have not been able to show by any simple means that the microscopic quantum mechanics rigorously reduces it to a two-mode model.

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†Consultant, Bell Telephone Laboratories, Murray Hill, N. J. 07974.

[1]Y. Toyozawa and J. Hermanson, Phys. Rev. Letters 21, 1637 (1968).

[2]Y. Toyozawa, in *Proceedings of the Third International Conference on Photoconductivities*, edited by E. M. Pell (Pergamon, New York, 1971), p. 151.

[3]P. J. Dean, D. D. Manchon, Jr., and J. J. Hopfield, Phys. Rev. Letters 25, 1027 (1970).

[4]A. S. Barker, Bull. Am. Phys. Soc. 16, 311 (1971).

[5]D. C. Reynolds, C. W. Litton, and T. C. Collins, Phys. Rev. B 4, 1869 (1971).

[6]D. C. Reynolds, C. W. Litton, T. C. Collins, and E. N. Frank, in *Proceedings of the Tenth International Conference on the Physics of Semiconductors, Cambridge*, 1970 (USAEC Division of Technical Information, Oak Ridge, Tenn., 1970), p. 519.

[7]C. H. Henry and K. Nassau, Phys. Rev. B 2, 997 (1970).

[8]K. Nassau, C. H. Henry, and J. W. Shiever, in Ref. 6, p. 629.

[9]C. H. Henry, K. Nassau and J. W. Shiever, Phys. Rev. B 4, 2453 (1971).

[10]W. Heitler, *Quantum Theory of Radiation* (Oxford U. P., London, 1957), p. 164.

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Electronic Properties of Graded Heterojunctions

Laura M. Roth and Alan J. Bennett
General Electric Research and Development Center, Schenectady, New York 12301

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A very simple one-band one-dimensional model, capable of extension to more realistic cases, is used to study the electronic properties of graded heterojunctions, in particular, their band edges, band gaps, and local densities of states. Explicit averages over the electron states calculated for various possible atom arrangements in the junction region are used to obtain these results. Clustering effects, inadequately treated in standard approximations, are found to be of crucial importance in determining the junction characteristics.

I. INTRODUCTION

In this paper, we study the electronic structure of graded heterogeneous interfaces; in particular, the band edges, band gaps, and local density of states in the junction region. These features are studied in optical[1,2] and conductivity[3] experiments. We use a very simple non-self-consistent one-band one-dimensional model, which when combined with impurity- and defect-level data does permit several predictions about the characteristics of three-dimensional multiband systems.

The concentration of species B in the region of an interface between a material composed of species A and one composed of species B increases from zero to the bulk B concentration over a distance characteristic of the particular materials and fabrication technique. At an interface between Si and SiO_2, for example, the junction can be schematically represented as $Si|SiO_x|SiO_2$, where the value of x varies over a distance of 10–20 Å from 0 in the bulk silicon to 2 in the bulk silica. The material in the intermediate region is, in general, a random, amorphous, and inhomogeneous alloy. As discussed in earlier work[4] the interface can be regarded as an alloy whose components are Si-Si bonds and Si-O-Si bridges.

Theoretical work on the electronic structure of inhomogeneous systems has been carried out by Gora and Williams[5,6] within the virtual-crystal approximation and using approximations suitable for composition variations over $\gtrsim$ 100 lattice distances. In this paper we shall deal with systems with widely differing components, in which the virtual crystal approximation is inadequate, and with more abrupt junctions.

We shall employ an explicit average over the electronic states calculated for various possible