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Band tailing in heavily doped semiconductors. Scattering and impurity-concentration-fluctuation effects

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Using a self-consistent multiple-scattering method, we estimate the relative importance of both effects of scattering and of impurity-concentration fluctuations on band states in heavily doped semiconductors and thus we account for band tailing. We apply this formalism to the estimate of the interband absorption spectrum in a typical case, in satisfactory agreement with experiment.

I. INTRODUCTION

A variety of experiments on doped semiconductors, most noticeably on their optical absorption, has given strong evidence for the existence of electronic states within an energy range extended into the band gap of the pure material, close to the band edges. The understanding of this band-tail-formation mechanism in a semiconductor, under the influence of charged impurities, has been a long-standing problem with both fundamental and practical bearings,[1] for which a comprehensive solution has not yet been found. Early approaches have considered the effect of scattering by impurities on electronic states, using perturbative methods.[2,3] Although the multiple-scattering method[2] was free of unsatisfactory approximations, it has not been numerically implemented to discuss the relevant experiments, presumably because it was not expected to give a tail in the density of states (DOS). On the other hand, approaches initiated by the work of Kane[4,5] have focused attention on the statistical properties of the scatterer distribution and yielded exponential tails in the DOS. These theories, however, come to the assumption that the electron energy fluctuations mirror those of the potential, forgetting about the scattering problem. These approaches have been widely used to discuss experimental data, although the actual width of the potential distribution which fits the experiment has usually been found to be significantly smaller than the theoretical one. Finally, Halperin and Lax[6] carried out an analysis which takes into account both the random distribution of impurities and the matching of the wave function to the local impurity distribution in a self-consistent manner; unfortunately, these results were restricted to the lowest-energy range of the band tail.

In the meantime, extensive studies of the electronic structure of disordered systems have made clear that any approach to this problem must incorporate both a *multiple-scattering* calculation of the electron Green's function and a *statistical* definition of this Green's function or of the associated self-energy. These points have been especially emphasized in Ref. 7. In addition, it is important, as stressed by Edwards,[8] to consider the actual disorder which an electron observes in the course of moving a mean free path. This suggests the analysis of the properties of a macroscopic-disordered system by averaging over the properties of microscopic neighborhoods.[9] The averaging procedure may be specified in terms of a sampling volume which depends on the electron energy through the energy dependence of the electron mean free path and which has to be estimated in a self-consistent way. Similar problems are encountered when one attempts to account for band-tail formation within the coherent-potential-approximation (CPA) formalism.[10]

On these grounds we present, in Sec. II, a self-consistent calculation of the band tail DOS in a doped semiconductor. We first estimate (Sec. II A) the effect of scattering by calculating the electron self-energy $\Sigma(\vec{k},E)$ via a renormalized perturbation expansion, assuming the impurity concentration to be homogeneous within the material; we thus account (Sec. II B) for the local fluctuations of impurity concentration. The relative importance of the scattering effect with respect to the local potential fluctuation one is thus estimated as a function of energy: we find the latter effect to play a role only in the lowest-energy part of the tail (Sec. III C). In order to make contact with the experiment and to assess the validity of our treatment, we present in Sec. III an analysis of a standard optical absorption spectrum[11] accounting for both the shift and the deformation of this spectrum with respect to the one of the unperturbed material. Here again, the relative importance of the scattering effect with respect to the one of impurity-concentration fluctuations is clearly displayed as a function of energy. Our results are summarized and further discussed in Sec. IV.

II. ELECTRON SELF-ENERGY AND DENSITY-OF-STATES CALCULATION

A. Effect of scattering

At the first stage, we consider free electrons in presence of a *homogeneous* distribution of donors (concentration N_D) and acceptors (concentration N_A) which scatter electrons through the Coulomb potential of their charge. We calculate the energy E and wave-vector $\vec{k}$-dependent self-energy

$$\Sigma(\vec{k},E)=N\sum_{\vec{k}'}\frac{|V_{kk'}|^2}{E-\epsilon_{k'}-\Sigma(\vec{k}',E)}. \tag{1}$$

In (1), $N=N_D+N_A$, ϵ_k is the unperturbed band energy, and $V_{kk'}$ the Fourier transform of the screened Coulomb potential

$$|V_{kk'}|=\frac{4\pi e^2}{\kappa|\vec{k}-\vec{k}'|^2}\,\frac{1}{\epsilon_{\text{TF}}(\vec{k}-\vec{k}')}=\frac{4\pi e^2}{\kappa[|\vec{k}-\vec{k}'|^2+q_s^2]}. \tag{2}$$

In (2), κ is the static dielectric constant of the matrix and the inverse screening length q_s, given by

$$q_s^2=\frac{4\pi e^2}{\kappa}\int_{-\infty}^{+\infty}\rho(E)\left(-\frac{\partial f}{\partial E}\right)dE,$$

depends on the actual density of states $\rho(E)$ and on the temperature, f being the Fermi-Dirac distribution function. For the sake of simplicity, we have used the Thomas-Fermi (TF) approximation for the wave-vector-dependent dielectric function ϵ, although more elaborate expressions (e.g., random-phase approximation) may be considered. Equation (1) corresponds to Klauder's third approximation (formula 63 of Ref. 2; see also Ref. 3). This is a high-density approximation in which, when one considers the scattering on a particular impurity, scattering on all other impurities are accounted for in terms of an effective medium (specified by Σ). An advantage of Klauder's approach is that it may incorporate series of diagrams of higher orders, in particular, those which would correspond to a bound-state formation. However, in Eq. (1) the latter diagrams are not included and thus we will limit our investigation to the doping range in which the bound-state formation is unlikely. Other contributions to the self-energy may be considered: the first-order Coulomb contribution vanishes for a homogeneous system[3] and, following Wolff,[3] we will approximate the exchange contribution by a constant term. Then, at a given N, the matrix integral equation (1) is iteratively solved for relevant E and k values; practically, we begin with the high-E values for which the convergence is fast. From Σ, we get the diagonal elements of the Green's function $G_{kk}(E)=G(\vec{k},E)=[E-\epsilon_k-\Sigma(\vec{k},E)]^{-1}$ and the DOS $\rho(E)=(\pi)^{-1}\operatorname{Im}G(\vec{k},E+i0)$. Let us notice that $\Sigma(\vec{k},E)$ is a complex quantity. In this respect, our method goes beyond the Brillouin-Wigner expansion, truncated to the second order. It also goes beyond the CPA-like methods which neglect the $\vec{k}$ dependence of Σ. Associated to Σ is a spectral density $C(\vec{k},E)$

$$C(\vec{k},E)=\operatorname{Im}\Sigma(\vec{k},E)\{[E-\epsilon_k-\operatorname{Re}\Sigma(\vec{k},E)]^2+[\operatorname{Im}\Sigma(\vec{k},E)]^2\}^{-1}. \tag{3}$$

At a given E, we may define k_m for which $C(\vec{k},E)$ is maximum. Taking the imaginary part of Σ as a measure of the damping of the quasiparticle, we may get an estimate of the E-dependent mean free path (mfp), $\Lambda(E)$:

$$\Lambda(E)=\hbar^2k_m/m^*\operatorname{Im}\Sigma(k_m,E),$$

where m^* is the effective mass of the unperturbed band. Obviously $\Lambda(E)$ as well as $\rho(E)$ depend on N.

B. Effect of impurity-concentration fluctuations

We have to take into account the statistics of the concentration fluctuations. We then face two problems. The first one is that, as in the discussion of the Anderson problem given in Ref. 7, Eq. (1) has to be understood as a self-consistent relation between the probability distributions for Σ on both sides of Eq. (1), given that the probability of having a local concentration N is $\mathcal{P}(N)$. As we have seen (Sec. II A), for a homogeneous impurity distribution, one was able to find a self-consistent solution for Σ. We will assume this solution to be still valid in a neighborhood, specified by its volume Ω, in which the impurity concentration is N; this approximation implies that an electron of the neighborhood is essentially scattered within Ω. We may then calculate a set of N-dependent DOS $\rho_N(E)$ and mfp $\Lambda_N(E)$. The second problem is to find $\mathcal{P}(N)$, given the mean value $\overline{N}$ of N. To this end, we will assume $\mathcal{P}(N)$ to be equal to the Poisson probability $\mathcal{P}(\nu)$ of having ν scatterers within a volume Ω; ν fluctuates around $\overline{\nu}$ with $\overline{\nu}=\overline{N}\Omega$:

$$\mathcal{P}(\nu)=(\overline{\nu})^\nu e^{-\overline{\nu}}/\nu!\,.$$

Clearly, the probability $\mathcal{P}(N)\equiv\mathcal{P}_\Omega(N)$ depends on Ω. By averaging the sets of $\rho_N(E)$ and of $\Lambda_N(E)$ with $\mathcal{P}_\Omega(N)$ we get, respectively, the average values of DOS $\overline{\rho}_\Omega(E)$ and of the mfp $\overline{\Lambda}_\Omega(E)$.

In Fig. 1 we have plotted, for different values of E, the variations of $\overline{\rho}_\Omega$ and of $\overline{\Lambda}_\Omega$ as a function of

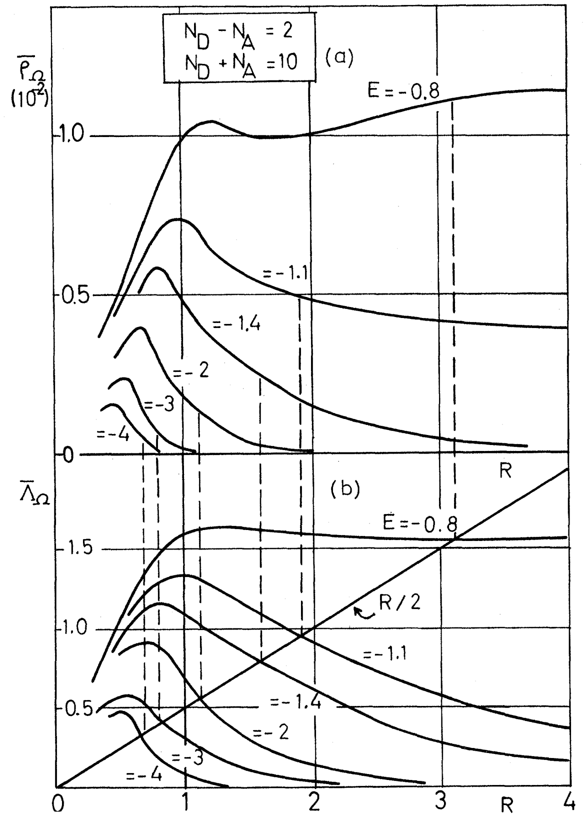

FIG. 1. Average values of (a) the density of states $\overline{\rho}_\Omega$ and of (b) the mean free path $\overline{\Lambda}_\Omega$ as a function of the radius R of the sampling volume Ω, for different values of energy E. The crossing of the straight line $R/2$ and of the Λ_Ω curves defines the self-consistent values of R. The vertical dashed lines which join the corresponding curves of (b) and (a) define the self-consistent density of states at a given energy. Energies are given in effective rydberg $\mathcal{R}^*$, lengths in effective Bohr radius a_0, density of states in states/$\mathcal{R}^* a_0^3$, and donor N_D and acceptor N_A concentrations in units of $\pi/3(4a_0)^3$.

the radius R of the sampling volume ($\Omega = \frac{4}{3}\pi R^3$); the calculations have been performed in a typical case, at $T = 0$ (which would correspond to, e.g., n-GaAs with $N_D = 1.2 \times 10^{17}$ cm^{-3} and $N_A = 8 \times 10^{16}$ cm^{-3}). Now, as pointed out by Butler and Kohn,[9] R cannot be smaller than about twice the mfp; on the other hand, by taking a larger radius, one underestimates the influence of the concentration fluctuations on the DOS. We have thus chosen to fix Ω from the self-consistent prescription

$$\Omega = \frac{4\pi}{3}[\mu \Lambda_\Omega(E)]^3 , \tag{4}$$

where μ is a constant ($\mu \gtrsim 2$). In actual calculations, we have taken $\mu = 2$, which gives an upper bound of the DOS in the tail; graphic solutions of Eq. (4) for different values of E are indicated in Fig. 1. The self-consistency requirement makes it clear that the incorporation of arbitrarily large fluctuations of N, which implies an arbitrarily small sampling volume and which would yield a DOS tail extending deeply in the band gap, corresponds to an unphysical averaging procedure. Calculations also show that, at high energy, the DOS becomes independent of Ω.

To summarize, we have shown that the E dependence of the sampling volume is essential and we have given a reasonable estimate of the DOS in the tail. The difficulty of the problem is less the taking into account of the impurity-concentration-fluctuation effect than the need to avoid overestimating it. Let us notice that our approach involves some approximations: for instance, we have assumed (i) the screening radius not to vary over the whole volume and (ii) any neighborhood to be electrically neutral (i.e., we have introduced no first-order Coulomb term in the local self-energy Σ).

C. Results and discussion

Our formalism deals with an isotropic, single-band semiconductor; however, it may be extended to any complex structure, for example, to the case of degenerate valence bands which is discussed below. For the case of an isotropic single band our results are universal and are best expressed in dimensionless units: energies and lengths are given in units of effective rydberg ($m^* e^4 / 2\kappa^2\hbar^2$) and of effective Bohr radius a_0 ($\kappa\hbar^2/m^* e^2$), respectively.

Results of DOS calculations are displayed in Fig. 2. We have considered the typical case discussed above which corresponds to an electron concentration, $N_D - N_A$, about twice as large as the critical one, n_c, for bound-state formation, n_c being estimated from $a_0 n_c^{1/3} = 0.25$. In Fig. 2(a) we have plotted, as a function of energy, the DOS calculated[12] (i) without taking into account the effect of impurity-concentration fluctuations [that is with Eq. (1), taking $N = \bar{N}$] and (ii) with incorporating this effect; in addition, we have plotted the unperturbed DOS and the one obtained from the Halperin-Lax tabulation.[6] Three features of these results are worth noticing. First, we properly describe the whole band-tail energy range: at high energy, the unperturbed DOS is recovered and, at the lowest energies, our results are close to those of Halperin and Lax. The agreement between the results of these authors and ours are hardly surprising for, if the calculations are very different, the starting demand (that is, to match the wave function or the Green's function to the local impurity configuration) is the same. However, data of Fig. 1 show that our de-

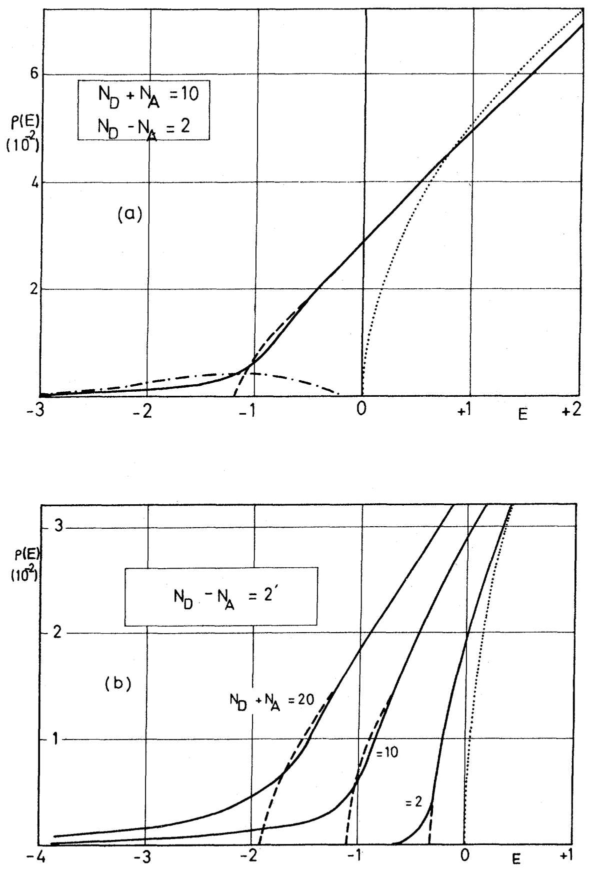

FIG. 2. (a) Density of states $\rho(E)$ as a function of energy. Full line, present calculations; dashed line, calculations omitting impurity-concentration-fluctuation effect; dotted line, parabolic band; dash-and-dot line, from Halperin-Lax tabulation. (b) Density of states as a function of energy for different degrees of compensation, keeping $N_D - N_A$ constant. Full line, present calculations; dashed line, calculations omitting impurity-concentration-fluctuation effect; dotted line, parabolic band. Units are those of Fig. 1.

finition of $\bar{\rho}_\Omega$, through the self-consistency relation (4), differs from the Halperin-Lax variational criterion which amounts to taking the maximum of $\bar{\rho}_\Omega$ as a function of R and which may imply a value of R smaller than twice the mfp. Second, we see in Fig. 2(a) that local concentration fluctuations lead to a finite DOS in the lowest-energy range for which the homogeneous scattering acting alone would give a vanishing DOS. Third, the effect of concentration fluctuations, namely, the difference between $\bar{\rho}(E)$ and $\rho_{\bar{N}}(E)$, is important only in the lowest-energy part of the band tail. In Fig. 2(b) DOS curves, calculated for various values of N_D and N_A, keeping $N_D - N_A$ constant, illustrate the effect of compensation.

III. OPTICAL ABSORPTION

We have used this formalism to analyze the deformation of the interband-absorption optical spectra in heavily doped semiconductors, this deformation being one of the clearest evidences of band-tail formation. The standard calculation of the optical absorption has to be modified to account for the fact that the spectral densities for the conduction and valence bands are no longer given by delta functions $\delta(E - \epsilon_k)$. In other words, to properly account for the wave-vector selection rule, we have to use the whole structure of the spectral densities. This point is worth emphasizing for most of the previously mentioned authors (see, e.g., Ref. 11) have merely assumed that the wave-vector selection rules were no longer holding in the band tail. The absorption coefficient α, at photon energy $\hbar\omega$, is given by

$$\alpha(\hbar\omega) = A \sum_v \int dE \int d^3k \, C^{(c)}(\vec{k}, E + \hbar\omega) C^{(v)}(\vec{k}, E) \times [f(E) - f(E + \hbar\omega)], \qquad (5)$$

where the sum runs over the light- and heavy-hole bands and where the constant A

$$A = \frac{e^2}{3\pi^3 c\omega} \frac{E_g(E_g + \Delta)}{(E_g + \frac{2}{3}\Delta) m_c \sqrt{\kappa}}$$

incorporates the interband optical matrix element for the zinc-blende structure.[13] E_g is the unperturbed gap energy and Δ the spin-orbit splitting which we have assumed to be independent of energy, c is the light velocity, and m_c the conduction-band effective mass. In Eq. (5), the presence of the Fermi function f accounts for the thermal occupation of the bands. The spectral function for the conduction band $C^{(c)}(\vec{k}, E)$ and for the light-hole and heavy-hold bands $C^{(vl)}(\vec{k}, E)$ and $C^{(vh)}(\vec{k}, E)$ are calculated using the formalism set up in Sec. II. In the calculation of $C^{(vl)}$ and of $C^{(vh)}$ and of the corresponding self-energies $\Sigma^{(v)}$, we have to account for both the intravalence-band and the intervalence-band transitions. As the approximation we use for the impurity potential matrix elements, $V_q = 4\pi e^2/\kappa(q^2 + q_s^2)$, involves plane waves rather than the actual Bloch functions, these matrix elements are the same for both transitions; this, as expected, introduces no splitting of the valence bands at $k = 0$. In addition, when considering a p-type material, we have to introduce into $\Sigma^{(v)}$ the exchange contribution Σ_x which we approximate by a constant term, proportional to $p^{1/3}$ (p being the hole concentration) and which is calculated at the Fermi level of the unperturbed system, taking the valence-band degeneracy into account.[3,11,14] The self-energies are then the same for both the heavy-hole and light-hole bands and given by

$$\Sigma^{(v)}(\vec{k},E)=\sum_{\vec{k}'}\frac{|V_{kk'}|^2}{E-\epsilon_k^{(l)}-\Sigma_x-\Sigma^{(v)}(\vec{k}',E)}+\sum_{\vec{k}'}\frac{|V_{kk'}|^2}{E-\epsilon_k^{(h)}-\Sigma_x-\Sigma^{(v)}(\vec{k}',E)},$$

where the dispersion relation for the unperturbed bands have been approximated by

$$\epsilon_k^{(l,h)}=\hbar^2k^2/2m_{l,h},$$

m_l and m_h being the light- and heavy-hole effective masses. Equation (5) contains no adjustable parameter; one readily verifies that the standard expression[15] for $\alpha(\hbar\omega)$ is recovered when one replaces $C^{(c)}$ and $C^{(v)}$ by δ functions (that is, at the limit of unperturbed bands). However, this treatment is still approximate in that, beside the electron-phonon coupling, it neglects (i) the so-called vertex corrections to the electron-hole Green's functions and (ii) the electron-hole Coulomb interaction.

We have considered the experimental results on (direct-gap) GaAs, thoroughly studied by Casey and Stern.[11] In what follows, we shall discuss the absorption spectrum of their Fig. 5 ($N_A=2\times10^{19}$ cm^{-3}, $N_D=4\times10^{18}$ cm^{-3}, $T=297$ K). Obviously, at a given energy E, the spectral densities $C(\vec{k},E)\equiv C_N(\vec{k},E)$ depend on N. To account for the effect of the local concentration fluctuations, we have to average the products $C_N^{(c)}C_N^{(v)}$ with the probability $\mathcal{P}(N)$:

$$\langle C^{(c)}(\vec{k},E)C^{(v)}(\vec{k},E)\rangle_{\text{av}}=\sum_N\mathcal{P}_\Omega(N)C_N^{(c)}(\vec{k},E)C_N^{(v)}(\vec{k},E),$$

the average having to be performed at each energy; at the lowest energy $\langle C^{(c)}(\vec{k},E)\cdot C^{(v)}(\vec{k},E)\rangle_{\text{av}}$ differs from $C_{\overline{N}}^{(c)}(\vec{k},E)\cdot C_{\overline{N}}^{(v)}(\vec{k},E)$. In the case of GaAs, owing to the larger values of the effective rydberg for the holes with respect to the one for the electrons, the shift of the valence bands with respect to the unperturbed band, that is the valence-band contribution to the gap shrinkage, is much larger than the corresponding term for the conduction band. For the same reason, the major contribution to the low-energy spreading of the band tail arises from the effect of concentration fluctuations on the valence band: This suggests approximating $\langle C^{(v)}(\vec{k},E)C^{(c)}(\vec{k},E)\rangle_{\text{av}}$ by $\langle C^{(v)}(\vec{k},E)\rangle_{\text{av}}C_{\overline{N}}^{(c)}(\vec{k},E)$.

In Fig. 3 are displayed the experimental data of Casey and Stern and the results of our calculations, together with the absorption curve calculated for an unperturbed system. The major features of the experimental spectrum are well reproduced by our calculations. First, with respect to the spectrum of the unperturbed system, we see a large shift of the absorption toward the lower energies; most of this gap shrinkage has its origin in the electron-impurity interaction. Second, at low energy there is a quasiexponential dependence of α as a function of $\hbar\omega$ which clearly differs from the usual power-law dependence of direct interband transitions. Let us notice that the electron-impurity interaction does not merely result in a translation of the absorption curve but rather in a deformation of the spectrum as seen from the fact that the curves for the perturbed system and for the unperturbed one almost coincide at high energy while they differ at low energy. We see that calculations are in close agreement with experiment from the highest absorption values down to $\alpha\sim500$ cm^{-1}; below this value, the theory still gives a fair agreement with experiment and does reproduce the shape of the band tail. We note that, at low energy, the comparison with experiment is less precise because (i) the figures of Casey and Stern involve the subtraction of an absorption term of 100 cm^{-1} which is ascribed by these authors to the free-carrier absorption and (ii) the absorption curve of a high-purity sample does exhibit, beside some excitonic structure, a tailing effect.[16]

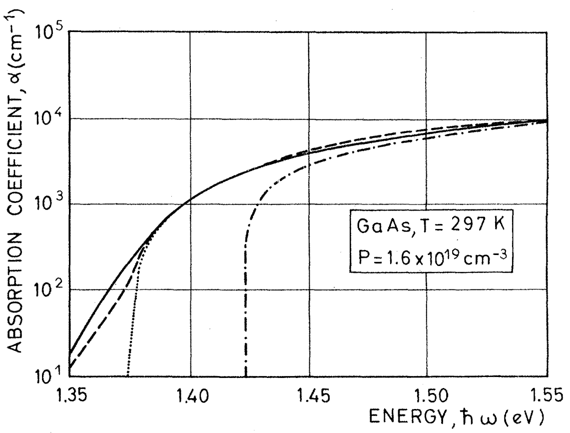

FIG. 3. Absorption coefficient α(cm^{-1}) as a function of photon energy $\hbar\omega$(eV) for a p-GaAs sample ($P=1.6\times10^{19}$ cm^{-3}; sample of Fig. 5, Ref. 11). Full line, experiment; dashed line, present calculations; dotted line, calculations omitting impurity-concentration-fluctuation effect; dash-and-dot line, unperturbed-band calculations.

In order to assess the relative importance of the effect of impurity scattering with respect to the one of concentration fluctuations, we have performed a calculation of the absorption spectrum in which we have used $C_{\overline{N}}^{(v)}(\vec{k},E)$ instead of $\langle C^{(v)}(\vec{k},E)\rangle$ that is, one in which the effect of fluctuations is suppressed. Results of these calculations, in Fig. 3, show that most of the deformation of the spectrum and of the gap shrinkage arises from the scattering effect and that the fluctuation effect is important only at the lowest energies. The agreement between our theory and experiment is far more significant in that calculations involve no adjusted parameter and the modification of the absorption spectrum includes both a shift and a deformation.

IV. DISCUSSION AND CONCLUSION

To summarize, we have presented a treatment of the band-tail formation in doped semiconductors which accounts for both effects of scattering and of statistical concentration fluctuations. In so doing, we have shown the relevance of the multiple-scattering method first proposed by Klauder and by Wolff, we have laid emphasis on the notion of average over neighborhoods suggested by Butler and Kohn, and we have incorporated in a self-consistent way the statistics of concentration fluctuations in the calculation of the average Green's function. Thus, we have proposed a solution to this long-standing problem within the spirit of recent theories of disorder. Our method yields the k- and E-dependent self-energies; this allows us to calculate the optical absorption spectrum and to show that its severe deformation may be accounted for in a nonempirical way. Our method would certainly be useful to discuss other properties (e.g., transport properties) of heavy doped semiconductors.

We have discussed the deformation of the optical absorption spectrum in doped semiconductors from the simplest viewpoint, that is, we have been merely calculating the band-to-band transitions. It is worth pointing out that this calculation which forgets about the influence of electron-hole interaction accounts for the major features of the spectrum and especially for the non-power-law behavior of the optical absorption at low energy, whereas the most common opinion is that this effect has not to be ascribed to a change in band-to-band transitions but to the deformation of the excitonic structure in presence of local potential fluctuations or of random electric fields: This is the exciton-breaking mechanism of Dow and Redfield.[17] In other words, we have shown that the perturbation of the one-particle excitation spectrum by charged impurities is of prime importance. Hopefully, our approach may offer a starting point for a more comprehensive discussion including the electron-hole interaction which is known, in some instances, to significantly modify the optical absorption.[18]

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