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IMPURITY WAVE FUNCTION AND ALLOY BROADENING OF IMPURITY-RELATED LUMINESCENCE*

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By performing state-of-art computations of the acceptor wave functions in GaAs we show that the linewidth of the conduction band to acceptor luminescence increases more than quadratically with the increase in the binding energy. This proves that study of the fluctuation broadening of the impurity-related emission in semiconductor alloys may provide a critical test for theories claiming realistic impurity wave function computation. The theoretical results are compared with the experimental data for high purity *p*-type AlGaAs alloys.

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In high purity *p*-type semiconductors, the low-temperature emission is dominated by bound exciton (BE) emission. At slightly lower energies transitions involving acceptors can be observed. The overlap between donor-acceptor transitions and transitions from the conduction band to acceptors (CA) can be mitigated by slight increase in temperature or pump level which favour the CA transitions.

The main difference between the emission processes in high-purity binary and ternary semiconductors is the occurrence of an additional emission broadening mechanism in the latter case, due to statistical fluctuations of the composition. These lead to a fluctuation of the band gap, and thus to a broadening of all electron-hole recombination processes. The magnitude of the fluctuations, and the resulting emission linewidth, increases with localization of the quasi-particles involved in the recombination. The linewidth of the BE emission is governed by the effective exciton volume, while for the CA emission it is the hole bound to an acceptor whose effective radius governs the linewidth. For the BE emission what counts is the composition dependence of a total energy gap (i.e., dE_g/dx). For the CA transitions only fluctuations of the absolute energy of the valence band (i.e., dE_{vb}/dx) are important. This is so because the mean free path of the electron recombining with a hole bound at an acceptor is much larger than the Bohr radius of the hole and the electron contribution to the broadening can be neglected.

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A quantitative theory of the alloy broadening requires precise definition of the effective volume V of the recombining quasi-particle. In previous approaches [1, 2] this has been rather arbitrary, which prevented the separation of the truly fluctuation limited broadening component of the experimentally observed linewidth from other sources of broadening. In our recent paper we showed, however, how this can be done qualitatively [3]. In case of the conduction-band to acceptor luminescence the emission half-width is

$$\Gamma = 2.35 \frac{dE_{vb}}{dx} \sqrt{x(1-x)} \int dr |\Psi(r)|^4, \quad (1)$$

where a numerical factor 2.35 comes from a Gaussian line shape of the emission and dE_{vb}/dx is the absolute composition shift of the valence band (band-offset). It is clear from above that even a small change in the acceptor wave function localization leads to large variation of the linewidth.

We have therefore computed the linewidth for several acceptors in AlGaAs by using a model that has recently been developed by one of us for the effective-mass acceptors in Si and Ge [4, 5]. Using this model, we computed the ground state energies and the values of the integral $I_4 = \int dr |\Psi(r)|^4$ for the effective-mass acceptors in GaAs and GaAlAs alloys. For the alloy we used the virtual crystal approximation with all relevant parameters linearly scaled between GaAs and AlAs (see Table 1 in Ref. [3] for a summary of the material parameters). We also retained the spherical symmetry of the Coulomb potential in the alloy. The major difference from the computations of the properties of acceptors in Si and Ge [4, 5] is that here we truncated the dielectric function into the dielectric constant ϵ_0 . The trial wave functions used in the computation were similar to those used in [4] and [5]. The binding energy of the acceptor computed by this method is 28.6 meV for GaAs. It favourably agrees with the experimental binding energy for the carbon acceptors (26.7 meV). In the alloy, the computed binding energies increase slightly faster with the Al content than the experimentally observed ones.

In Fig. 1 we compare the best published results of the CA emission linewidths Γ_{CA} in the direct-gap $Al_xGa_{1-x}As$ alloy with those computed by the realistic model of the acceptors in AlGaAs alloy and a crude hydrogenic model. In the latter a certain estimation of the spherical Bohr radius a_B which used in computing the integral I_4 was made through the relation $E_b = e^2/2\epsilon_0 a_B$. The binding energy in the alloy taken from Ref. [6] changes with Al content x as $E_b = (26.7 + 5.75x + 123x^{3.4})$ meV.

It is well known that the shallow impurity binding energies depart from the predictions of a model which assumes a purely Coulomb potential of the defect. A good example is provided by simple acceptor in GaAs for which about 50% change of the binding is observed (Fig. 2). The deepening of the impurity level results in the wave function contraction, and in consequence with the increase in alloy broadening. To estimate the magnitude of the effect we used the numerical computation based upon the model outlined above, but adding an extra localized term in the impurity Hamiltonian

$$V = Ae^{-\alpha r} \quad \text{with} \quad \alpha = 1 \text{ a.u.} \quad (2)$$

Here A is a parameter, whose change produces various chemical shift. For each

Fig. 1. Comparison of the best published results of the CA luminescence half-widths in $\text{Ga}_{1-x}\text{Al}_x\text{As}$ (taken from [7] $\circ$, [8] $\square$, [9] $\triangle$, [10] $\diamond$ and [11] $\star$) with theory (full curve — simplified hydrogenic model, full symbols $\blacksquare$ — realistic model of acceptors and dashed line — theory of Ref. [1], but with updated material parameters).

Fig. 2. The dependence of the relative alloy broadening on the acceptor ionization energy calculated within: the realistic theory (full curve) and the hydrogenic model (dashed-dotted line).

value of A the normalized wave function is computed, as well as the value of the I_4 integral. The relative change of broadening for a given acceptor is determined by the square root of the ratio of the I_4 integral for this acceptor to the value of $I_{4,C}$ for carbon — the most Coulomb-like acceptor among all.

In a crude hydrogenic model the Bohr radius is proportional to $1/E_b$, and thus

$$\Gamma(E_b) = \Gamma_C(E_b/E_C)^{3/2}. \quad (3)$$

The predictions of both models are summarized in Fig. 2. The expected changes for the four shallowest acceptors (i.e. C, Be, Mg and Zn) are not large and may escape experimental detection. However, for the deepest acceptors the increase

is much more dramatic: an about twofold increase in the emission linewidth for Si and a threefold for Ge. This is why a careful study of the fluctuation broadening of the acceptor-related emission in low-doped high quality semiconductor alloys may provide a critical test for theories claiming realistic impurity wave function computation. The above effect (second-order effect) is much more sensitive than a simple comparison of the experimental energy data with the computation of the energy shifts (a first-order effect).

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