Random-Alloy Splitting of Cu Levels in $GaAs_{1-x}P_x$

In a recent Letter, Samuelson *et al.*[1] reported new peaks in the luminescence spectra of Cu-doped $GaAs_{1-x}P_x$ alloys which differ from the single peak observed for the binary GaAs:Cu. They interpreted them as due to levels related to the substitutional Cu_{Ga} centers with different local environments: They observed in the alloys three peaks that they could correlate with the nearest-neighbor configurations surrounding the Cu atoms (i.e., 4As, 3As-1P, 2As-2P). In this Comment, we compare these data with those published for excitons bound to substitutional N_P centers in $Ga_{1-x}In_xP$:N alloys where similar interpretations have previously been given.[2,3] We mention also a quantitative approach that we presented recently,[4] which allows us to calculate the energy difference between localized levels split in an alloy by the different local configurations surrounding the defect core. We apply this model successfully to the Cu_{Ga} centers in $GaAs_{1-x}P_x$:Cu alloys.

In GaP:N, an isolated nitrogen impurity locally binds an exciton, the radiative recombination of which gives rise to a very narrow luminescence line. When one adds a small amount of indium to the GaP binary, three *different* luminescence bands appear in $Ga_{1-x}In_xP$:N, which are specific to these alloys.[3] By comparison with GaP:N and $GaAs_{1-x}P_x$, we attribute them to the recombination of excitons bound to nitrogen surrounded by different local configurations: We proposed that these excitons were mainly sensitive to the first-nearest neighbors of the N centers, i.e., that they reveal the 4Ga, 3Ga-1In, 2Ga-2In configurations. There are two differences which exist between these older results and the new ones presented in Ref. 1. (i) For $GaAs_{1-x}P_x$:Cu, the luminescence peak intensities are proportional to the statistical occurrence of each configuration under the assumption of a random distribution of the Cu atoms in the alloy matrix, while this is *not* the case in the $Ga_{1-x}In_xP$ luminescence spectra. By comparing these latter data with the excitation spectra (that only reveal the local density of states), we showed that this was due to the efficient transfer which occurs from N sites of high energy to N sites of low energy. These transfer processes were recently observed by measuring the time-resolved luminescence spectra of these N-excitons bands.[5] (ii) The energy difference between two alloy-split levels is 10–15 meV for $Ga_{1-x}In_xP$:N,[3] while it is 35–40 meV for $GaAs_{1-x}P_x$:Cu.[1] These differences explain why these alloy-split levels appear more clearly in $GaAs_{1-x}P_x$:Cu.

To account for the energy splitting between these levels, we proposed an embedded-cluster calculation. This theoretical approach was developed in order to consider the local environment effects on the electronic spectra of a short-range-potential impurity in substitutional alloys.[4] The method describes both alloy potential fluctuations around the impurity (i.e., the different local configurations), and the self-consistent alloy effective medium, using a simple density-of-states shape for the binary limits (semielliptic band). We found with this formalism an energy difference $\Delta E = 12$ meV between the exciton levels due to nitrogen surrounded by 4Ga and 3Ga-1In, and $\Delta E = 14$ meV between the next two nitrogen local density-of-states contributions, in good agreement with the experiments. For $GaAs_{1-x}P_x$:Cu, with assumption of a semielliptic valence band with average values for the holes in GaP and GaAs, and from knowledge of the Cu levels in the two binaries, we were able to find an energy splitting $\Delta E = 40$ meV between each interval of two different Cu levels in the alloy. These results correspond to the experimental data reported by Samuelson *et al.*[1] Therefore, from our experience with nitrogen as a local probe in $Ga_{1-x}In_xP$:N alloys, copper in $GaAs_{1-x}P_x$ appears to be an even better local configurational probe in the respect that it gives rise to a random-alloy splitting of the Cu levels three times larger than that due to nitrogen in $Ga_{1-x}In_xP$:N.

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