Comments

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Comment on "Comprehensive analysis of Si-doped $Al_xGa_{1-x}As$ ($x=0$ to 1): Theory and experiments"

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The experimental data reported by Chand *et al.* [Phys. Rev. B **30**, 4481 (1984)] agree qualitatively with the deep levels and shallow-deep instabilities predicted by an intervalley effective-mass theory (IVEMT) originally proposed by Resca and co-workers. Furthermore, the experimental data do not agree with an alternative IVEMT proposed by Altarelli and Hsu and Chang, McGill, and Smith. The latter theory predicts only shallow substitutional donors. In interpreting the experimental data, Chand *et al.* use an IVEMT that follows the scheme of Resca and co-workers: An impurity pseudopotential is introduced with a cutoff radius and the intervalley kinetic energy term is effectively dropped. However, a clear discussion of the role of such a term in the calculations by Chand *et al.* is missing.

The intervalley effective-mass theory (IVEMT) used in the theoretical section of the paper by Chand *et al.*[1] leaves some important questions unanswered. The authors use the theory to interpret their experimental observation of a large increase in the activation energy E_d of a silicon donor level in $Al_xGa_{1-x}As$ that occurs at alloy concentrations corresponding to direct-indirect band-gap crossover. A different analysis of experimental data of this type has been proposed by Schubert and Ploog[2] which does not require such large increases in E_d. However, there seems to be little doubt that a donor level associated with equivalent multivalley X or L minima is deep, whereas a donor level associated with a single-valley Γ minimum is shallow. The occurrence of both kinds of phenomena was first predicted, and consistently maintained, by Resca and co-workers.[3–9] Experiments of the kind performed by Chand *et al.* in which one varies the alloy composition or in which an applied stress is used to induce an inequivalent band-minima crossover were explicitly proposed in the last sections of Refs. 6 and 7. In an alternative IVEMT Altarelli and Hsu[10,11] and Chang, McGill, and Smith[12] have consistently argued that such a shallow-deep instability should not occur for substitutional donors, and that only shallow levels are predicted. Deep substitutional chalcogen donors in Si (Refs. 7–9 and 13) and in Ge (Ref. 14) have subsequently been confirmed experimentally. The basic question of the existence of those deep ground-state levels has not been discussed by Altarelli.[15]

The experiments of Chand *et al.* fit within the scheme of Resca *et al.*[6,7] However, Chand *et al.* claim to use the alternative IVEMT of Altarelli *et al.*[10,11] and Chang *et al.*[12] to predict deep levels and shallow-deep instabilities. This is in opposition to the general conclusions of all previous work on the alternative IVEMT.[10–12] The point at issue is whether an intervalley kinetic energy term should be included in a correct IVEMT or not. Chand *et al.* restrict their comments on this point to a footnote (Ref. 29) of their paper.[1] From the footnote it appears that the authors have discarded the intervalley kinetic energy term. On the other hand, a cutoff in the impurity pseudopotential is used in the paper. This is precisely the basic point of the work by Resca *et al.*, who have shown that the introduction of the intervalley kinetic energy term is erroneous,[6] whereas the use of a cutoff in the impurity pseudopotential is necessary.[3–9] On the other hand, Altarelli and Chang *et al.* have argued that an intervalley kinetic energy term must be included, and it is precisely this factor which prevents the occurrence of shallow-deep instabilities.[11,12] In fact, Herbert and Inckson[16] had previously shown that, if included, an intervalley kinetic energy term dominates all others with increasing wave-function localization, thereby preventing the occurrence of shallow-deep instabilities. In another paper on GaP, Chang *et al.*[17] include the intervalley kinetic energy term and find only shallow levels. They then empirically double the calculated umklapp renormalization factor R_2 to account for an even moderately deep level.

At this point one concludes that Chand *et al.* have in fact applied the scheme of Resca *et al.*[18] However, in their footnote (Ref. 29) Chand *et al.* state that after having done a variational calculation without an intervalley kinetic energy term and with a cutoff potential, they evaluate the intervalley kinetic energy term and find it to be negligible. This contradicts previously cited results[11,12,16] in which a much stronger point-charge potential is controlled by the large intervalley kinetic energy term, which prevents the occurrence of the shallow-deep instability. One might believe that the $Al_xGa_{1-x}As$ alloys are drastically different than the previously studied perfect crystals, but this is unlikely. The simultaneous occurrence of deep levels and multivalley band minima now appears to be a quite general phenomenon, and the occurrence of a number of shallow-deep instabilities has been directly linked to the intervalley scattering mechanism. The most reasonable observation is that the intervalley kinetic energy term is extremely difficult to calculate and approximations have been taken to reduce its strength.[12] Perhaps Chand *et al.* use an even more severe truncation to make the intervalley kinetic energy term completely negligible in this work.

Finally, the paper by Chand *et al.*[1] suggests that the IVEMT has quantitative predictive value for the deep-donor binding energies. In fact, the IVEMT can only predict the onset of a shallow-deep instability from the shallow side and cannot quantitatively predict the binding energies of deep levels due to a number of severe approximations. This is true for elemental semiconductors such as Si (Refs. 3–9) and even more certainly for an alloy in which band and mass interpolations are taken, inequivalent band minima cross over, and strong local-field effects due to partial ionicity cannot be neglected in the dielectric screening.[19] The reason why Chand *et al.* achieve an apparent quantitative agreement between the IVEMT and the experimental data for the deep-level binding energies may be that, in addition to the potential cutoff radius, an interpolated effective mass is used as a parameter. The binding energies of the IVEMT in the region of a shallow-deep instability are very sensitive to small variations of most parameters and an apparently insignificant change in an effective mass may produce large changes in the predicted deep-donor binding energies. However, the reader should be warned that this is not a real quantitative prediction of the deep-donor binding energies.

In conclusion, a convincing discussion of the central role of intervalley kinetic energy in an effective-mass theory that predicts deep levels and shallow-deep instabilities in $Al_xGa_{1-x}As$ is missing in the paper by Chand *et al.*[1]

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