Monte-Carlo Model for Hole Mobility in $GaAs_{1-x}Bi_x$

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Dilute Bismuth alloy of GaAs, or $GaAs_{1-x}Bi_x$ is getting attention these days because of its peculiar properties [1], [2]. This material is a good candidate for use in optical devices such as infrared detectors, used in communications systems, as well as spintronics and solar cells [3], owing to a stable band gap in a temperature-varying environment [4], as well as the variability of the band gap with that of alloy percentage over the manufacturable range of 0% to around 6%. The latter is a property that can be exploited for the purpose of material engineering and making optical devices for different wavelengths. The band gap reduction as compared to intrinsic GaAs happens due to change in valence bands because of the presence of Bismuth states slightly below the valence band maximum (VBM). These states couple with the three spin-degenerate valence bands, namely heavy, light, and split-off hole bands, resulting in a band structure configuration that is significantly different from that of intrinsic GaAs.

In this paper, we study the transport behavior of $GaAs_{1-x}Bi_x$ alloy material and its potential application using Monte-Carlo simulation with respect to variation in alloy percentages as well as the doping concentration. Our model is based on two main components. First is the Valence-band anti-crossing model [3], [5] for incorporation of Bi states and their coupling with valence bands of GaAs. This k.p based model produces a band structure which is shown in Fig. 1, compared with intrinsic GaAs. We can see the incorporation of two Bismuth levels -0.4 eV and -1.9 eV result in flattening of the curvatures of the bands and hence increased effective masses. In addition, these levels shift the VBM upwards, as seen in the figure, resulting in band gap reduction that is proportional to the alloy percentage. The second component of our model is the Monte-Carlo (MC) based simulation, a well-known technique to study transport behavior of materials with known band structure or effective masses, and scattering rates, with results that are more realistic compared to drift-diffusion and hydrodynamic based approaches. We use our model for a range of Bi alloying percentages, as well as doping concentrations.

We have used the GaAs scattering rates, [6] corrected for the ionized-impurity scattering, [7] and the addition of alloy scattering due to the presence of Bi [8]. Fig. 2 shows mobility values for intrinsic GaAs and Bi-alloyed GaAs for doping concentrations ranging from 10^{14} cm^{-3} to 10^{19} cm^{-3}. The results for GaAs match well with those in reference [9]. Bi concentration is fixed at 5% in this calculation. The Bi mobility is decreased compared to intrinsic GaAs for all values of doping concentration. This is due to the effect of the band structure modification, resulting in increased effective masses, as well as presence of alloy-scattering. Fig. 3 shows the mobility of $GaAs_{1-x}Bi_x$ for values of x ranging from 1% to 6%. The impurity doping concentration was kept constant at around 3×10^{17} cm^{-3}. We see that the mobility drops from the intrinsic GaAs value for increasing Bi concentration. This can be compared with the experimental values recently obtained by Beaton et. al [10], and Kini et. al [11].

We intend to show detailed results regarding our model as applied to this material as well as discuss its implications and possible future directions related to the technology.

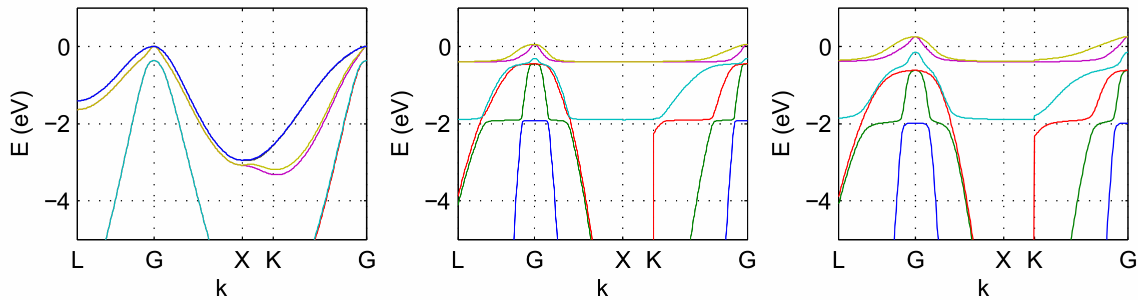

Fig. 1. Band-structure plots for intrinsic GaAs, 1% $GaAs_{1-x}Bi_x$ and 6% $GaAs_{1-x}Bi_x$

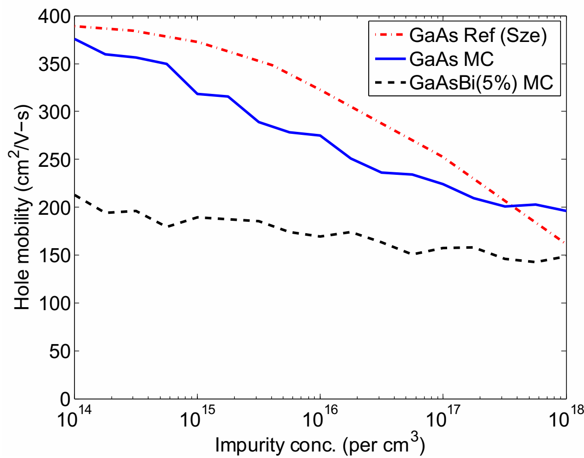

Fig. 2. Hole mobility vs impurity concentration for intrinsic GaAs (ref. and sim.) and $GaAs_{1-x}Bi_x$ sim.

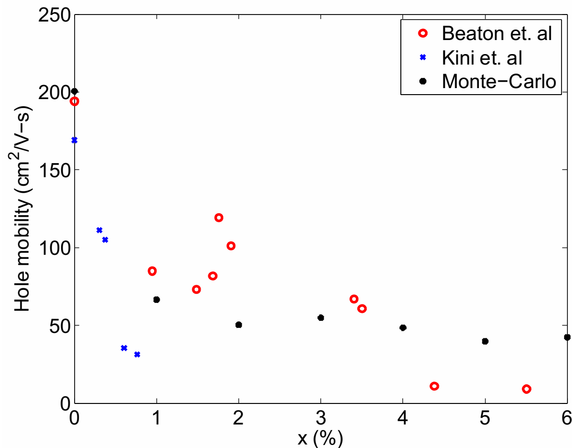

Fig. 3. Hole mobility vs x in $GaAs_{1-x}Bi_x$, for our model compared with experiments.

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