Modelling the Auger Recombination Rates of $GaAs_{(1-x)}Bi_x$ Alloys

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***Abstract*—We calculate the |Conduction, Heavy Hole (HH)⟩ - |Split-off Hole (SO), HH⟩ (CHSH) Auger Recombination rates for $GaAs_{(1-x)}Bi_x$ alloys, which are candidates for highly efficient telecommunication devices. A ten-band, tight-binding method, including spin-orbit coupling, was performed on a 9x9x9 strained supercell in order to generate an accurate band structure to perform the calculation on. This band structure was then unfolded to give a true E-k relation. As predicted by experiment, there should be a decrease in the Auger recombination rate as the concentration of Bismuth increases ending in a suppression at greater than ~11% Bismuth.**

I. Introduction

Recent studies have shown that dilute Bismides offer a simple control of the size of the band gap and sharp reduction in non-radiative Auger recombination rates [1]. Most studies focus on $GaAs_{(1-x)}Bi_x$ alloys, which have a band gap in the region of the telecommunications spectrum, and are highly relevant for a variety of optical devices requiring improved efficiency. However, experiment can only give an idea of the effect of bismuth on Auger recombination rate, therefore, a better picture, of how the recombination rates vary with bismuth concentration, will be essential in the development of these devices.

Introducing bismuth has been shown to reduce the band gap and simultaneously increase the HH-SO gap (ΔE_{so}), which implies the weakening of the transition strength between the SO and HH bands. This is the transition that causes recombination to become non-radiative and is a dominant loss mechanism at telecommunications wavelengths. Currently, attaining ΔE_{so} which is larger then the band gap, E_g, which would supress the CHSH Auger recombination rates, is difficult to achieve. This is thought to be at ~10.5% bismuth concentration, however, recent growth techniques have only successfully achieved ~6%. Therefore it becomes important to know the dependency of recombination rates at lower bismuth concentrations.

II. Modeling

A. Unfolding Supercell Band structure

Using the tight-binding method on a supercell structure allows strain and defects to be integrated into the band structure. It also allows you to recreate specific characteristics of materials within the structure including clustering which is a common growth problem in dilute Bismides. All these effects are very important for GaAsBi because of the strong role played in altering the dispersion relation with changing bismuth concentration. However, these supercell calculations come at a price.

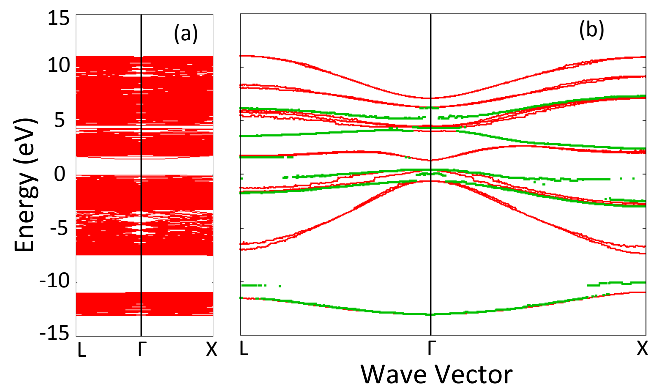

Fig. 1. The (a) folded and (b) unfolded band structure of a 9x9x9 GaAsBi supercell structure at 10% bismuth. Green lines represent defect bands introduced by bismuth.

A supercell brillouin zone is smaller than that of a primitive cell, yet holds more information. Due to, this reduction in k-space volume, the band structure information is folded into the supercell brillouin zone. In this folded form, the band structure becomes nearly impossible to analyse due to the density of bands which can be seen in Fig. 1a. There is also no longer a true E-k relation because the energies are folded to a false k-position.

Using the unfolding method highlighted by Boykin and Klimeck [2], the band structure in Fig. 1b was generated giving an effective primitive cell dispersion relation but retaining the supercell characteristics. This E-k relation is then far simpler to run the Auger recombination calculations on.

B. Auger Recombination

Auger recombination is where the energy from an electron hole pair recombining is passed through a virtual photon and excites a second electron. In the case of CHSH recombination in lasers, this leads to a decrease in efficiency since the conduction band electrons and Valance band holes do not always recombine radiatively and hence requires a larger threshold current to increase the number of radiative recombinations.

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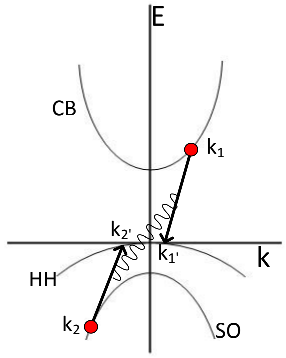

Fig. 2. CHSH Auger recombination showing the first electron, k_1, recombining with hole, k_1, passing its energy to the second electron, k_2, which in turn recombines with hole, k_2.

The rates can be considered by the transition probability and the occupancy (or valency with respect to holes). This is given in (1)

$$R = 2\left(\frac{2\pi}{\hbar}\right)\left(\frac{4\pi e^2}{\epsilon}\right)\frac{1}{(2\pi)^9}\int dk_1 \int dk_{1'} \int dk_2 \cdot |M|^2 \theta \delta(\Delta E_1 - \Delta E_2) \quad (1)$$

where before the integral is simply a constant prefactor. $\delta(\Delta E_1 - \Delta E_2)$ conserves energy and $k_{2'}$ is chosen so that momentum is conserved. gives the occupancy (valancy) of the electron (hole) states based on Fermi statistics. $|M|^2$ represents the transition matrix and is given by [3]

$$|M|^2 = \left|\frac{\langle k_1 \mid k_{1'}\rangle\langle k_2 \mid k_{2'}\rangle}{|k_{1'} - k_1|^2} - \frac{\langle k_1 \mid k_{2'}\rangle\langle k_2 \mid k_{1'}\rangle}{|k_{2'} - k_1|^2}\right|^2 + \left|\frac{\langle k_1 \mid k_{1'}\rangle\langle k_2 \mid k_{2'}\rangle}{|k_{1'} - k_1|^2}\right|^2 + \left|\frac{\langle k_1 \mid k_{2'}\rangle\langle k_2 \mid k_{1'}\rangle}{|k_{2'} - k_1|^2}\right|^2 \quad (2)$$

where $|k_i\rangle$ represents the eigenvector of electron, i, and $|k_{i'}\rangle$ represents the eigenvector of hole, i.

There is only a small range of k in which (1) needs to be solved because, outside this range, the contribution is negligible.

III. Conclusion

The calculated CHSH Auger recombination rates are expected to show a decreasing trend with increasing bismuth concentration as predicted from both the theory, with respect to band movements, and experiment. A sharp rise in the recombination rate should be found at ∼10.5% Bismuth concentration which is due to $E_g \approx \Delta E_{so}$. This increases the number of direct transitions that can occur where transitions without a transfer of momentum are far more likely. Finally, the Auger recombination rates beyond this point are expected to be negligible.

These results will advance the knowledge of the relationship between Bismuth concentration and the associated loss mechanisms, which will assist in the development of a balance between reducing defects and increasing efficiency.

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