Vacancy Effects on Optical Gap in GaAs in The Presence of Spin Orbit Interaction

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Abstract— **We calculate the band structure of the Ga As in the presence of vacancy, in the effective mass approximation (EMA) by using virtual crystal approximation based on an 8-band kp formalism. For the calculations shown, the Hamiltonian constructed by Trebin et al. has been implemented. This 8-band kp Hamiltonian is constructed solely on group theory arguments and, when applied correctly, guarantees the inclusion of all matrix elements compatible with the Td symmetry group of the zincblendes up to the desired order in the electron wave vector k.Finally we have calculated energy gap in various wave vector K versus vacancy percent . It is shown that by increasing vacancy percent the band gap energy is decreased. So we can control optical properties of this mater by changing vacancy percent**

I. INTRODUCTION AND BACKGROUND

The role of disordered GaAs is of importance from two points of view; first in growth process of a GaAs some impurities and vacancies are created, the second one is its application in industry and electronic devices.The electronic band structure of ternary compound semiconductor is of considerable theoretical and experimental interest.[1,2] The study of the optical constants, requires derivation of band structure. The optical constant has applications such as interference filters, optical fibers, and reflective coating that requires accurate knowledge of their optical constants over a wide range of wavelengths. Second, the optical properties of crystalline matters are related to their electronic band structure.The interest in electro-absorptive effects in quantum-well structures is strongly motivated by their potential applications in a variety of electro-optic devices such as high speed modulators[3], self-linearized modulators [4], wavelength selective detectors[5], and optically bistable switches[6]. Also in spin based electronics, an efficient spin polarized current is much demanded. There have been a number of researches demonstrating spin injection from dilute magnetic semiconductors or ferromagnetic metals into semiconductors.[7-8] In recent researches the use of conventional nonmagnetic semiconductors at zero magnetic field, has obtained a spin polarized current in resonant tunneling heterostructure. Perel et al. proposed that using a material which lacks the center of inversion as a barrier for electron tunneling can produce a considerable spin polarization, such as zinc-blende structure semiconductors [9]. They showed using a single barrier heterostructure only Dresselhaus spin-orbit interaction makes the spin polarization efficiency of about 20%. Thus there exists a need for more accurate models to calculate the electronic band structure of disordered material. Here by using virtual crystal

approximation (VCA) we calculate the band structure, in the effective mass approximation (EMA) [10] based on an 8-band $k\cdot p$ formalism . There are several published 8-band $k\cdot p$ Hamiltonians[11], each including a more or less detailed set of effects. For the calculations shown, the Hamiltonian constructed by Trebin et al. [12] has beenimplemented. This 8-band $k\cdot p$ Hamiltonian is constructed solely on group theory arguments and, when applied correctly, guarantees the inclusion of all matrix elements compatible with the T_d symmetry group of the zincblendes up to the desired order in the electron wave vector k. This method to construct $k\cdot p$ Hamiltonians was first outlined by Luttinger and developed generally by Bir and Pikus. This model calculate the band structure in the presence of spin orbit interaction and this Hamiltonian arising from the lack of inversion symmetry of bulk zincblendes, or the BIA terms. The inclusion of the BIA terms allows a more faithful reproduction of the D_{2d} or C_{2v} symmetry of the [001] resonant tunneling structures. In bulk zincblendes, the BIA terms cause a lifting of the spin degeneracy away from the Brillouin zone center.

II. RESULTS

The conduction band spin splitting in a two-band model can be described by the following Hamiltonian[12].

$$H = \eta_D \sum_{i=1}^{3} \sigma_i k_i \zeta_{ijk} (k_j + k_k)(k_j - k_k)] \qquad (1)$$

where

$$\zeta_{ijk} = \begin{cases} 0 & i = j \ \ or \ \ i = k \ \ or \ \ j = k \\ 0 & i = j = k \\ 1 & otherwise \end{cases} \qquad (2)$$

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η_D describes the strength of the Dresselhaus phenamenon, the σ_i's are the Pauli matrices and the K_i's are the electron wave vector component. To use prefect-crystal techniques to approximate the energy bands of the mixture materials ,one must use a model for the matter which is periodic. One of the simplest models , the "rigid-band model," is very useful when the concentration of one component (solvent) is much larger than the concentrations of other component (solutes). Here we think about vacancy such as atomes with zero on-site energies and calculate the band structure in the presence of spin orbit interaction. we have calculated energy gap in various wave vector K versus vacancy percent It is shown that by increasing vacancy percent the band gap energy is decreased. So we can control optical properties by changing vacancy percent.

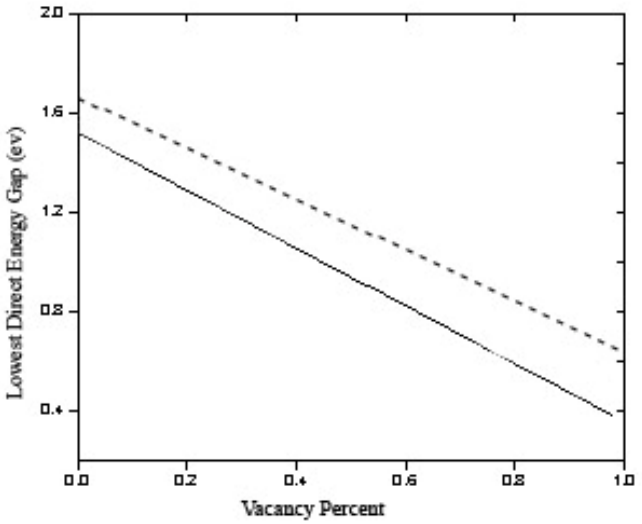

Figure.1. The lowest direct energy gap of GaAs as a function of vacancy percent. Solid line is plotted for K=0, dash line is $K=0.04\times 2\pi/a$.

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