ELECTRONIC STRUCTURE OF III - V TERNARY AND QUATERNARY ALLOYS

BY

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Dedicated

to

My Parents

CERTIFICATE

This is to certify that the Thesis entitled "Electronic Structure of III-V Ternary and Quaternary Alloys" which is being submitted by Miss V.B. Gera for the award of Degree of Doctor of Philosophy to the Indian Institute of Technology, Delhi, is a bonafide record of research work carried out by her under our guidance and supervision.

The results have reached the standard, fulfilling the requirements of the regulations relating to the degree. The results submitted in this Thesis have not been submitted to any other university or institute for the award of any degree or diploma.

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ABSTRACT

The electronic band structure of III-V substitutional alloys calculated within the framework of coherent-potential approximation (CPA) and tight-binding formalism are presented. The major advantage of semiconductor alloys over binary compounds is that the semiconductor alloys extend the opto-electronic properties in the spectral region intermediate to two constituent compounds. The III-V semiconductor alloys studied presently are the anion substituted ternary alloys $GaAs_{1-x}P_x$ and $InAs_{1-x}P_x$, the cation substituted ternary alloys $Ga_xIn_{1-x}P$ and $Ga_xIn_{1-x}As$, and the quaternary alloys $Ga_xIn_{1-x}As_yP_{1-y}$ lattice-matched to InP and GaAs as well as the quaternary $Ga_{0.5}In_{0.5}As_{0.5}P_{0.5}$.

The disorder in substitutional semiconductor alloys arises due to the random distribution of atoms at lattice sites, so that the translational symmetry does not exist in substitutional alloys. The disorder-induced effects have been computed within coherent-potential approximation which is treated as the best single-site approximation. The disorder in the diagonal atomic term values has been treated in CPA, while the off-diagonal disorder has been treated in virtual crystal approximation (VCA).

Band structure calculations have been performed using tight-binding method where the interactions upto and including second neighbor have been taken into account. The spin-orbit interactions have been taken into account explicitly. Tight-binding parameters of Porod et al. [J. Vac. Sci. Technol. 21,

965 (1982)] reproduce all the important gaps of involved binaries - GaP, GaAs, InP and InAs, which agree very well with the recent experimental data.

Partial s and p cation as well as anion density of states (DOS) have been computed using sampling procedure. Calculation of partial CPA self-energy Σ from partial VCA DOS is an iterative procedure starting from the value of $\Sigma = 1/4(\Delta - i\Delta)$, where Δ is the alloy scattering parameter. The real part of the complex CPA self-energy gives correction to VCA band structure, while its imaginary part gives life-time broadening effects.

The complex energy band structure of the ternary alloys $GaAs_{0.5}P_{0.5}$, $InAs_{0.5}P_{0.5}$, $Ga_{0.5}In_{0.5}P$ and $Ga_{0.5}In_{0.5}As$, where the disorder is expected to be maximum, are studied in detail. In addition, the variation of seven important states - Γ_{15v}, Γ_{1c}, X_{5v}, X_{1c}, X_{3c}, L_{3v} and L_{1c} as a function of composition x is studied for all the four ternary alloys in the whole composition range between two end-point semiconductors. It is found that CPA self-energy correction is maximum for cation s-like states. The variation of direct as well as indirect Γ-X and Γ-L energy gaps with composition x is studied within CPA for all these alloys. The calculated variation of these gaps is seen to match well with the available experimental data. The CPA bowing parameter is found to be small for anion substituted ternaries - for $GaAs_{1-x}P_x$, the calculated value is 0.177 eV, while for $InAs_{1-x}P_x$, it is 0.035 eV. For cation substituted ternary alloys, the calculated bowing is found to be large - it being 0.7 eV for $Ga_xIn_{1-x}P$ and 0.79 eV for $Ga_xIn_{1-x}As$. These values agree with the experimental data.

A crossover between the direct gap and indirect Γ-X gap has been obtained for the ternary alloys $GaAs_{1-x}P_x$ and $Ga_xIn_{1-x}P$. The alloy $GaAs_{1-x}P_x$ is found to be a direct gap semiconductor for $0 < x < 0.5$ and an indirect gap semiconductor for $x > 0.5$. For $Ga_xIn_{1-x}P$ alloy, the crossover is obtained at $x = 0.77$, it being an indirect gap semiconductor for $x > 0.77$. Finally, the variation of E_1-optical gap with composition x is studied for all the ternary alloys, and a good agreement between theory and experiment has been obtained.

The CPA technique has also been applied to enumerate the electronic properties of the quaternary alloy $Ga_xIn_{1-x}As_yP_{1-y}$. The complex energy band structure of the quaternary alloy $Ga_{0.5}In_{0.5}As_{0.5}P_{0.5}$ is studied. The compositional variation of direct as well as the indirect Γ-X and Γ-L gaps has been studied for the quaternary alloys $Ga_xIn_{1-x}As_yP_{1-y}$ lattice-matched to InP and GaAs. The bowing parameters calculated in VCA as well as in CPA for various values of x and y are presented for both the lattice-matched quaternary alloys. The disorder-induced effects are seen to be larger for GaAs lattice-matched quaternary than for InP lattice-matched one. This is also found to be true for the E_1-optical gap which has been calculated for the various combinations of x and y. The compositional variation of direct gap and E_1-optical gap for the InP lattice-matched quaternary is seen to agree with the experimental values.

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