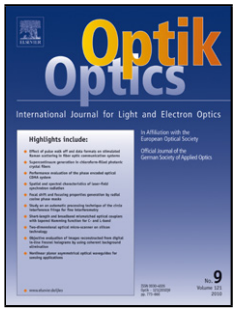

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A structural and electronic property of GaAs and Ge and super-lattice GaAs / Ge (001)

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ABSTRACT

The structural and electronic properties of the bulk GaAs and Ge semiconductor and the band offsets for the GaAs/Ge and AsGa-Ge interfaces are investigated by density functional theory (DFT). This calculation has shown that the lattice parameter is underestimated by the local density (LDA) approximation and overestimated by the generalized gradient approximation (GGA). An opposite behavior is observed for the bulk modulus B_0. Concern, the super-lattice GaAs/Ge (001), studied in our work, we found that the substitution of the atom of the interface affects the discontinuity of the VBO valence band, which is mainly due to the different electronic charges accumulated in the interfaces.

Keywords: DFT; ; ; ; ; , LDA, GGA, Structure bands, density of States, VBO.

I. Introduction

The germanium, semiconductor crystallizes in a diamond-like structure. It was operated in the technology as a semiconductor substrate until the silicon takes its place at the onset of the years 60. Nowadays, it is more used in the fabrication of photovoltaic cells and it is also found in the state of an alloy with Silicon (Ge-Si). The GaAs, semiconductor, crystallizes in a zinc blende structure which is characterized by high mobility of carriers and a direct band gap necessary for the optical transitions to be effective. For this reason their field of applications is well developed in rapid microelectronic **[1]**.

Semiconductor–semiconductor interfaces play a crucial role in modern electronic and optoelectronic devices **[2]**. The transport properties in superlattice devices are controlled by the electronic band profiles at the interfaces, more specifically by the valence discontinuities that accommodate the difference in band gap between the materials, namely, the valence band offsets (VBO). We calculate the different interfaces by considering semi-infinite semiconductors, and discuss the limit of a thick interlayer by analyzing separately the Ga-Ge and As-Ge ideal interfaces. Although this thick covalent limit does not seem to be stable **[3]** [in the sense that the energy will be lowered by substituting atoms in few interface layers to have mixed AsGa-Ge or mixed GaAs-Ge layers which give a compensated (neutral) interface], it is worth discussing this limit as a check to the calculations for a thin covalent interlayer

In order to determine the physical properties of a semiconductor and the valence band offsets of a superlattice, extensive experimental and theoretical work in the past few years has tried to achieve and understand that tuning, using different approaches.

It is possible to study the energetic and the electronic structure of many-electron systems by performing fully ab-initio computations. Among the existing ab-initio schemes, the local-density approximation and