**Zeitschrift:** Helvetica Physica Acta
**Band:** 62 (1989)
**Heft:** 6-7

**Artikel:** Valence-band offset at InP/Ga_0.47In_0.53As lattice-matched heterojunctions

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**DOI:** https://doi.org/10.5169/seals-116134

# VALENCE-BAND OFFSET AT $InP/Ga_{0.47}In_{0.53}As$ LATTICE-MATCHED HETEROJUNCTIONS

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**Abstract:** The valence-band offset of $InP/Ga_{0.47}In_{0.53}As$ interfaces has been computed for the (001), (110) and (111) orientations. The offset is 0.30 eV independent on the orientation and results from competing anion and cation additive contributions.

## 1. Introduction and methods

The valence-band offset (VBO) at $InP/Ga_{0.47}In_{0.53}As$ lattice-matched heterojunctions has been studied theoretically by applying the first-principles pseudopotential method to periodically repeated supercells containing 3 double layers of each material and using the virtual-crystal approximation for the GaInAs alloy. The selfconsistent electron density of the supercell is used to obtain the electrostatic potential lineup $\Delta\overline{\overline{V}}$, that is the difference between the average Hartree potential in the two materials. The VBO is then obtained by adding to $\Delta\overline{\overline{V}}$ the difference $\Delta E_v$ between the bulk valence-band edges calculated at equal value of the average Hartree potential. Details of the methods are in [1].

## 2. Results and conclusions

For the (001) orientation we calculate $\Delta\overline{\overline{V}}=-0.25$ eV, due to the interface dipole which is evident in the macroscopic average [1] of the electron density reported in Fig. 1(a). Given that $\Delta E_v=+0.55$ eV (which includes the spin-orbit but not the self-energy corrections) we obtain a VBO of +0.30 eV, to be compared with the recently measured value $0.35\pm0.01$ eV [2].

In order to investigate separately the anion and the cation discontinuities, we consider the ideal heterojunctions CP/CAs and InA/XA, where $X=\langle Ga_{0.47}In_{0.53}\rangle$ and $C=\langle In_{0.5}X_{0.5}\rangle$, $A=\langle P_{0.5}As_{0.5}\rangle$ are the reference virtual cation and anion

respectively. The total interface dipole in Fig. 1(a) is nothing but the superposition of the competing anionic and cationic dipoles present in CP/CAs and InA/XA heterojunctions, and correspondingly the total electrostatic potential lineup can be decomposed as $\Delta\overline{\overline{V}} = \Delta\overline{\overline{V}}_C + \Delta\overline{\overline{V}}_A = (+0.36 - 0.61)$ eV.

Fig.1(b) shows the macroscopic average of the electrostatic potential of the (001), (110), and (111) interfaces. Although at the interface the profile is sensitive to structural details (different interference between the anionic and cationic dipoles), $\Delta\overline{\overline{V}}$ is the same for the three orientations, prooving that in this isovalent system the VBO is orientation independent, as already found for GaAs/AlAs [1].

Finally, we construct the InP/XAs interface from the reference periodic crystal CA by transforming the virtual anions A into P or As depending on the site and similarly for the cations C. It is the electronic response to this perturbation which produces $\Delta\overline{\overline{V}}$and, within linear theory, it is given by the superposition of the linear response (LR) to each monoatomic substitution. From a computation of the latter [3] we obtain $\Delta\overline{\overline{V}}_{\rm A}^{(LR)} = -0.58$ eV, $\Delta\overline{\overline{V}}_{\rm C}^{(LR)} = +0.34$ eV and so that the $\Delta\overline{\overline{V}}^{(LR)} = -0.24$ eV, in excellent agreement with the SCF supercell result.

## 3. References


[1] A. Baldereschi, S. Baroni and R. Resta, Phys. Rev. Lett. **61**, 734 (1988).

[2] D. V. Lang et al., J. Sci. Vac. Technol. B **5**, 1215 (1987).

[3] M. Peressi, S. Baroni, A. Baldereschi, and R. Resta, to be published.


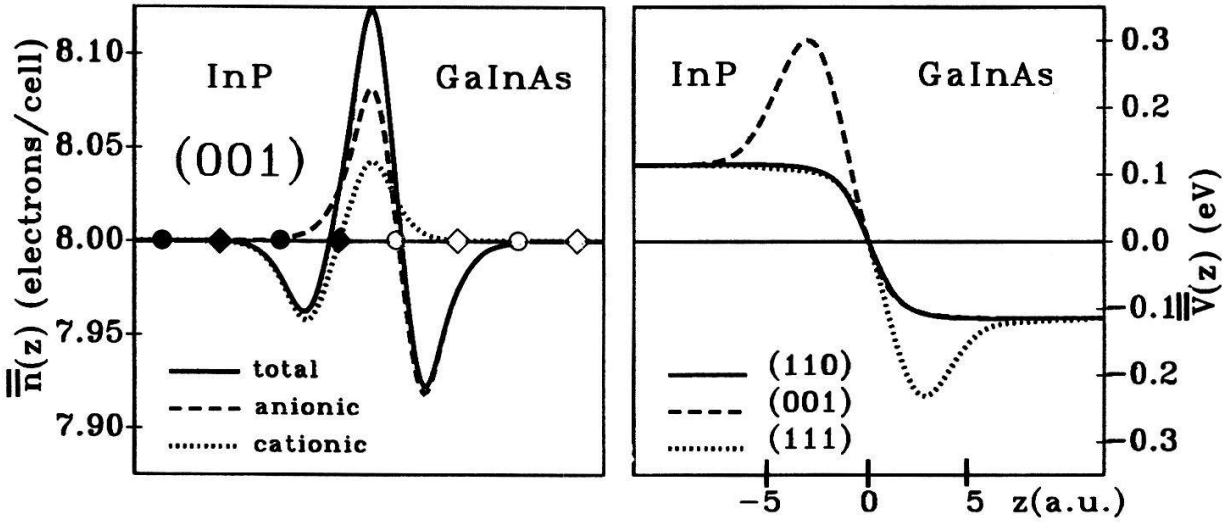


**Fig.1.(a):** Macroscopic average $\overline{\overline{n}}(z)$ of the electron density in $InP/Ga_{0.47}In_{0.53}As$ (001), and its decomposition into anionic and cationic contributions; circles (squares) indicate the position of the cation (anion) planes. **(b):** Macroscopic averages $\overline{\overline{V}}(z)$ of the electrostatic potential for (001), (110) and (111) interfaces; the origin is choosen where $\Delta\overline{\overline{V}}$ equals the average of the two bulk values.