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CHARGE TRANSFER VS. ENERGY LEVEL PINNING AT SEMICONDUCTOR INTERFACES

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Abstract:

We investigate model assumptions concerning the physical mechanisms which determine the lineup, and in particular we study Tersoff's argument from a first-principle viewpoint. The relevance of local fields to the potential lineup problem is discussed.

1. Introduction

The important parameters which govern optical and transport properties at semiconductor heterojunctions are the valence and conduction band-edge discontinuities. Essentially two kinds of model theories exist for predicting band offsets: one focuses on charge density information [1,2] and the other is based on the pinning of a suitable reference level [3,4]. Tersoff's argument for lattice-matched semiconductor heterojunctions states that if there is a discontinuity in the bare ionic potential across the interface, then the electrons will readjust such as to screen that jump with the macroscopic dielectric constant. Since typical bare jumps are of the order of 0.5 eV and $\epsilon \approx 10$, the final lineup will be ≈ 0.05 eV. Then, looking for the analogue of the metal Fermi level, Tersoff defines for each bulk material an effective midgap point E_B through a cell-averaged real-space Green's function. E_B is the energy where valence and conduction bands contribute equally to this function. The final self-consistent offset is approximated through lining up the effective midgap energies.

2. Results and conclusions

A novel ab-initio approach [5] has been proposed recently to deal with the problem of band offset at semiconductor heterojunctions. The actual interface is treated as a perturbation with respect to a virtual periodic crystal, and the interface electronic charge is shown to be very well described by first-principles linear-response theory. In order to check Tersoff's argument about macroscopic screening of potential discontinuities, we have performed supercell calculations for GaAs/AlAs (110) and GaAs/Ge (110) heterostructures. We used density functional theory in the local-density approximation, 12 atoms in the unit cell, local Berkeley pseudopotentials and a kinetic

energy cutoff of 14 Ry. In order to subtract bulk effects and to blow up interface features we use the concept of *macroscopic average* [2,5] (see Figure 1).

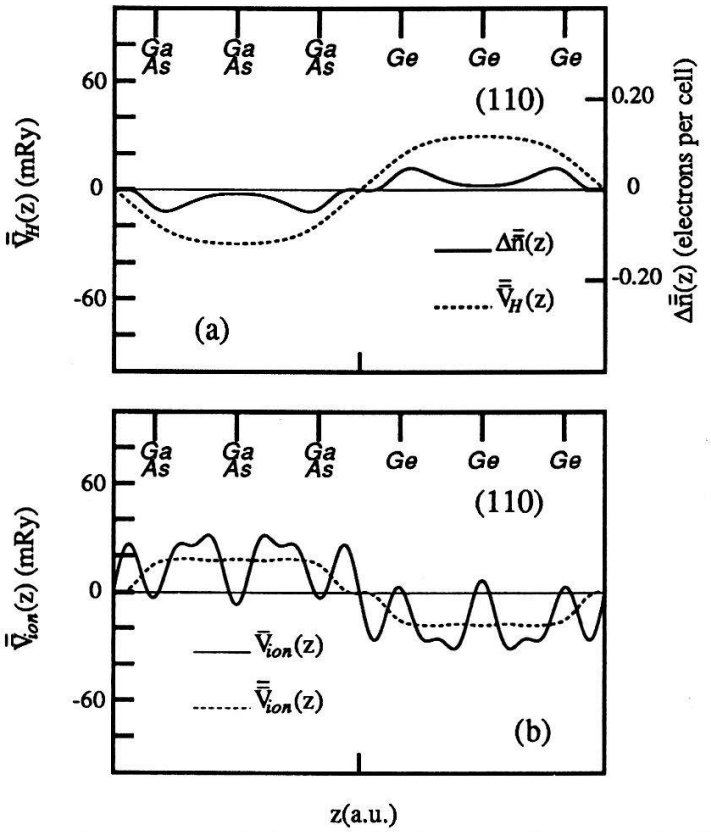

Figure 1: (a): Macroscopic average of electron density and Hartree potential for the (110) GaAs/Ge interface. (b): Planar and macroscopic averages of the bare ionic perturbation.

Our calculations show that —contrary to the basic assumption underlying reference-level model theories— local-field effects [6] cannot be always neglected. We arrive at the following results for GaAs/Ge: $\Delta\ \bar{\bar{V}}_{ion} = 0.50$ eV (see Figure 1(b)); $\Delta\ \bar{\bar{V}}_H =$ -0.79 eV (Figure 1(a)) and for the total self-consistent potential $\Delta\ \bar{\bar{V}}_T =$ -0.29 eV. Our results suggest that there are cases where *local-field effects* are negligible (this happens *e.g.* in GaAs/AlAs), and the total SCF pseudopotential is a good reference level there. But in general local-field effects could contribute to the offsets some tenths of an eV.

3. References

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