Structure of the As Vacancies on GaAs(110) Surfaces

S. B. Zhang and Alex Zunger
National Renewable Energy Laboratory, Golden, Colorado 80401
(Received 16 January 1996)

We report a comprehensive study of the As vacancies (V_{As}) in the GaAs(110) surface via *ab initio* total energy minimization. Previous scanning tunneling microscopy (STM) images of the V_{As} in p-type GaAs(110) were interpreted with a structure with outward movement of the Ga next to the vacancy. While our simulation of the STM images, using *ab initio* wave functions, agrees with experiment, our total energy minimization suggests, however, inward movement of Ga. We explain this apparent conflict as a charge induced band bending effect. As a consequence, we predicted that the STM images will depend on the applied bias voltage. We show that the atomic geometry of the surface $V_{As}(q)$ depends critically on the charge state q in sharp contrast with *bulk* vacancy. [S0031-9007(96)00556-X]

PACS numbers: 68.35.Dv, 61.16.Ch, 71.15.Nc, 73.20.–r

The electronic and atomic structures of point defects on surfaces could differ significantly from their bulk counterparts. For *bulk* As vacancy (V_{as})

TABLE I. Direction of atomic displacements (↑ - outward, ↓ - inward, ↔ - little displacement) near an As vacancy in GaAs(110). TB and PS stand for tight-binding and pseudopotential total energy calculations

	From total energy minimization			From STM images	
Site	TB (Ref. [2])	PS (Ref. [3])	PS (Present)	Expt. (Ref. [2])	Calc. (Present)
As	?	?	↔	↓	↓
Ga	↑ s0.7 Åd	↓ s≤0.4 Åd	↓ s0.3 Åd	↑ s0.7 Åd	↑ s, 0.6 Å[a]d

[a]Inferred from the calculated dsplacement s0.4 Åd with respect to the third nn Ga atom and the measured [2] displacement of the third nn Ga and Ga distance away s0.2 Åd.

ϵ_{VBM}). The last term in Eq. (1) accounts for the energy of the n electrons or holes in the reservoir. Assuming that L_i is the supercell's ith dimension where i - x, y, and z (z is normal to the surface) and that Δz - $z_2 - z_1 \ll L_z$ can be any interior, bulklike region of the GaAs slab, ϵ_{VBM}, in principle, can be determined [1] by aligning the average potential

$$\overline{V} - \frac{1}{L_x L}$$

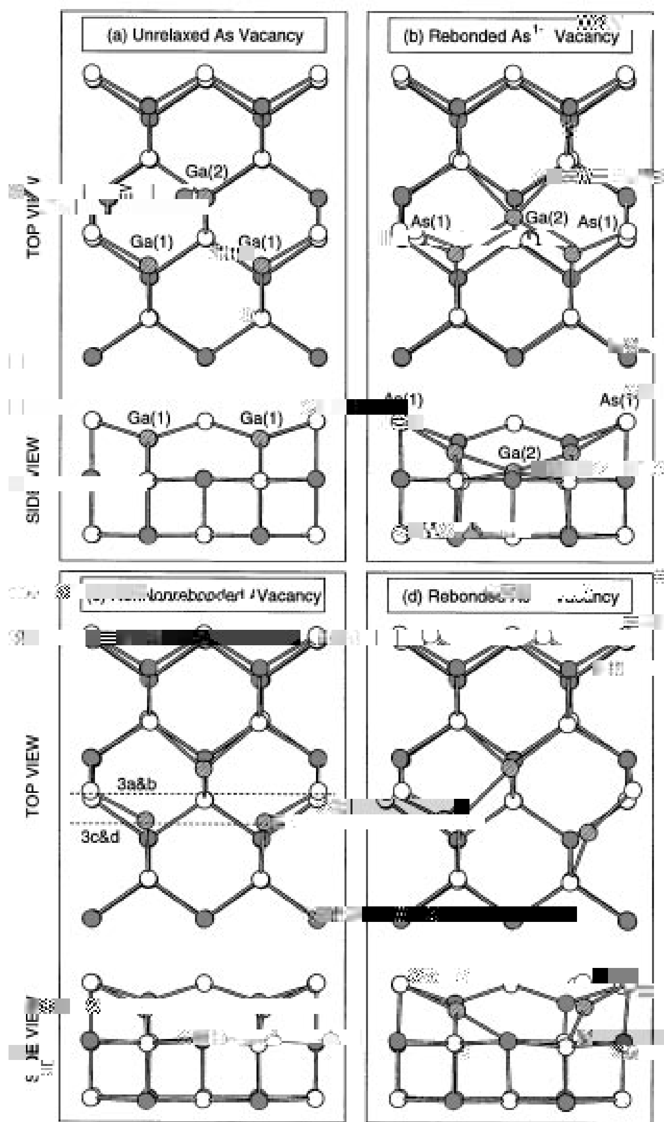

FIG. 1. Top and side views of the relaxed GaAs(110) surface

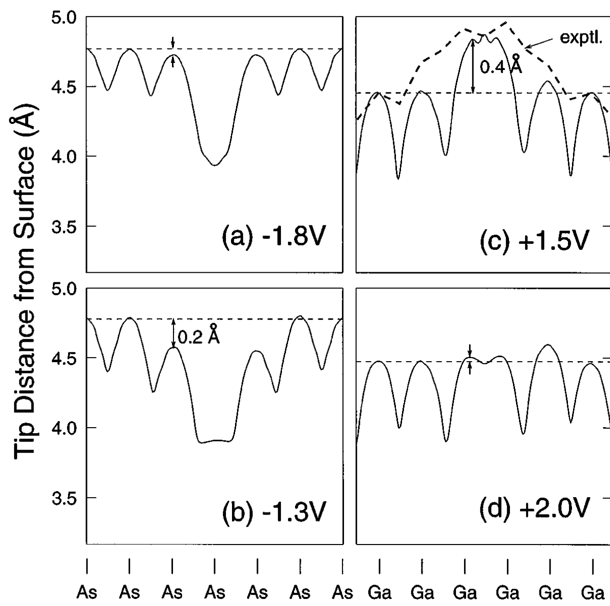

FIG. 3. Cross sections [see Fig. 1(c)] of the calculated 3D STM images at various biases for the nonrebonded V_{As}^{1+} center. The experimental data in (c) are taken from Ref. [2] and are aligned with the calculated results at the third nearest neighbor