model, Cowley, Cochran, Brockhouse, and Woods[7] and Kunc, Balkanski, and Nusimovici[5] found that the former does not have any term corresponding to the $\underline{T}\underline{S}^{-1}\underline{\tilde{T}}$ term of the latter. With the SEC term due to the deformation dipoles included, there is now a complete correspondence between the second-order energy expressions of the two models. A term-by-term comparison of Eq. (5) with the corresponding equation of the shell model gives the following physical meanings to the various shell-model matrices:

$$\underline{\varphi}^s = \underline{R}, \quad \underline{\tilde{m}}(\underline{\alpha}^d)^{-1}\underline{m} = \underline{T}\underline{S}^{-1}\underline{\tilde{T}},$$

$$\underline{\alpha} = \underline{Y}\underline{S}^{-1}\underline{Y}, \quad m = -\underline{Y}\underline{S}^{-1}\underline{\tilde{T}},$$

where the shell-charge matrix $\underline{Y}$ and the shell and core force-constant matrices $\underline{R}$, $\underline{S}$, and $\underline{T}$ are in the notation of Ref. 5. From these relations one finds that

$$\underline{\alpha} = \underline{\alpha}^d = \underline{Y}\underline{S}^{-1}Y.$$

Thus the general shell model corresponds to a special form of the new deformation dipole model in which $\underline{\alpha} = \underline{\alpha}^d$.

In conclusion, based on Zeyher's microscopic theory of lattice dynamics of ionic crystals, I have written down an expression [Eq. (5)] giving the second-order energy for the most general deformation dipole model including the SEC term due to the deformation dipoles not present in Hardy's model. The general shell model is similar to a special form of the new deformation-dipole model.

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GaSb Surfaces States and Schottky-Barrier Pinning*

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Photoemission measurements on GaSb indicate no surface states in the band gap. Deposition of Cs to form a Schottky barrier on *n*-GaSb moves the Fermi level 0.55 eV and produces pinning within the band gap. Thus, for the first time, Schottky-barrier pinning without the presence of intrinsic surface states in the gap is directly demonstrated.

Surface-state studies of clean, cleaved (110) GaSb and of cesium on (110) GaSb are reported. These results which represent work on two cleaves of an n-type[1] and one cleave of a p-type GaSb crystal are in disagreement with recent results published by Eastman and Freeouf[2] (EF) and modification of their generalizations concerning Schottky barriers appears necessary.

Figure 1 shows the high-energy portions of photoelectron energy distribution curves (EDC's) for clean and cesiated n-type (carrier concentration 1.1×10^{18} cm^{-3}) and clean p-type (carrier concentration 1.6×10^{17} cm^{-3}) (110) GaSb at an incident photon energy of 10.2 eV. In Fig. 1, a Cs monolayer is defined as the coverage which gives minimum photoemission threshold.[3] Further experimental details are available elsewhere.[3,4] The EDC's are presented with the peaks due to direct transitions in the bulk superimposed. Fermi-level positions determined to within ± 0.1 eV using a Cu reference emitter are marked near the high-energy edges. The difference in energy of the positions of the Fermi level on the clean n- and p-type samples is 0.65 eV, which is almost the full band gap. An additional determination of the n-type Fermi level based on yield measurements and the observed width of the EDC of the clean sample is in agreement with Fig. 1, putting the

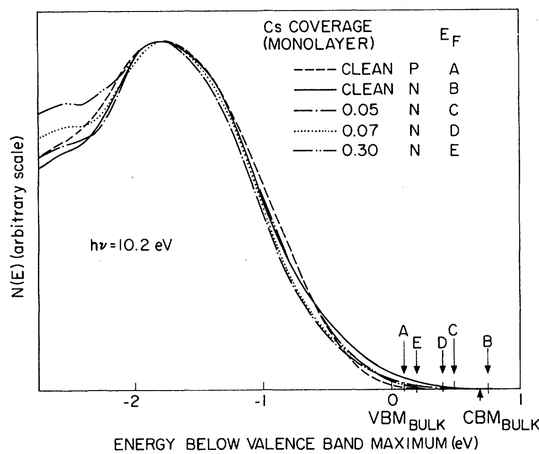

FIG. 1. The high-energy portions of clean- and cesiated-GaSb EDC's; $h\nu = 10.2$ eV. The Fermi level (E_F) of the n-type sample shows a large movement with cesiation and the Fermi levels of the clean p- and n-type samples differ in energy by 0.65 eV. This shows that the Fermi level of the n-type sample lies near the conduction-band minimum and indicates the absence of empty intrinsic surface states which would cause pinning.

surface Fermi level, E_F, on n-type GaSb at the conduction-band minimum (CBM). This corresponds to a flat-band situation with the forbidden band gap free of empty intrinsic surface states which would cause pinning. EF, on the other hand, showed empty surface states on GaSb as having a peak near the CBM with a tail extending below midgap and located the Fermi level on their n-type sample 0.4 eV below the CBM.

Further evidence for the intrinsic n-type Fermi-level location being near the CBM is given by following the Fermi-level movement with Cs addition. It is evident that with cesiation the Fermi level moved towards the valence band maximum (VBM) and eventually moved through the band gap by 0.55 eV and stabilized near the VBM,[5] in accordance with the Fermi-level position for bulk Schottky barriers.[6] If the intrinsic Fermi-level position on an n-type sample were located about 0.4 eV below the CBM as reported by EF, such a large movement would be impossible.[7]

It appears possible to reconcile the present results with those of EF. Lapeyre and Anderson[8] have suggested that excitonic effects may be important in the Ga $3d$ transition used by EF to detect their empty surface states. This would result in a measured empty-surface-state position appreciably below that of its true energy, and could explain the difference between EF's location of the empty surface states using photoemission partial-yield spectroscopy and our results.

There is a large variation reported in the literature for the surface Fermi-level position on cleaved GaSb. Viljoen, Jazzar, and Fischer[9] found a variation of 0.6 eV across the surface of a newly cleaved sample with E_F finally stabilizing at 0.1 eV above the VBM after several days. EF found E_F to lie about 0.3 eV above the VBM. As is described below, we believe that these pinning positions have been affected by the unusually high sinsitivity of GaSb E_F to oxygen (and presumably other gases). Recent studies of the effects of oxygen on clean GaSb by Chye *et al.*[10] show that the position of E_F can be affected by quite small amounts of oxygen. Movement is seen even at 10^{-5} Torr sec O_2 exposure. At 10^{-2} Torr sec O_2 the E_F moved downward by about 0.5 eV. Sensitivity to other gases might be even greater.[11]

With use of MacRae and Gobeli's sticking probability of less than 10^{-5} for oxygen,[12] these exposures correspond to less than 10^{-4} and 10^{-1} monolayer coverage, respectively. In agreement with MacRae and Gobeli's low sticking probability, no structure due to oxygen was found in the EDC's ($h\nu \leq 11.6$ eV) for these exposures. We therefore suggest that this unusually high sensitivity of E_F to exposure to oxygen (and presumably other gases) is due to the lack of any intrinsic-surface-state pinning. In GaAs[13] and InP[14] where empty intrinsic surface states were present in the band gap no such sensitivity was found.

The present work shows that surface-state pinning may be produced at a metal-semiconductor contact even when empty intrinsic surface states are not present. It also shows that the Fermi-level pinning position may be far removed from the bottom of the conduction as well as the empty surface-state band when these surface states lie in the conduction band. Thus, it appears that the conclusion of EF that intrinsic surface states play a predominant role in determining Schottky barriers in III-V semiconductors must be reexamined. In particular, their conclusion seems only clearly applicable when empty surface states lie in the band gap. The present work shows directly for the first time that Schottky-barrier pinning can be obtained in the gap even when no intrinsic surface states lie in the gap.

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