III. SEMICONDUCTOR SURFACE STUDIES

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1. ELECTRONIC STRUCTURE OF HOMOPOLAR AND HETEROPOLAR SEMICONDUCTING SURFACES

Joint Services Electronics Program (Contract DAAB07-76-C-1400)

John D. Joannopoulos, Eugene Mele

We are interested in the intrinsic and extrinsic surface states at surfaces of Group IV, III-V, and II-VI semiconductors. In these studies we are using a theorem we developed which reduces the semi-infinite surface system to an effective one-dimensional problem that can be solved with transfer matrix techniques. The electrons are studied with realistic tight-binding Hamiltonians which provide an attractive and physical real-space description of the states.

Specifically, we have recently studied the effects of bad cleaves on surfaces of GaAs (110). The results explain the strange behavior of the Fermi level position as a function of cleave quality for both n-type and p-type samples. In addition, the effects of O and O_2 adsorbates on GaAs (110) have been studied. Previous conflicting experiments regarding the nature and position of the oxidation process have been resolved. Finally, the nature of a semiconductor-metal interface is being studied. A new ionicity scale is introduced that accounts for the remarkable covalent-to-ionic behavior of Schottky barriers with metal work functions.

2. SURFACE PHONONS IN BONDED SOLIDS

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John D. Joannopoulos, Robert B. Laughlin

The nature of surface phonons in bonded solids is being investigated. Particular attention to disordered systems with large internal voids is given. These materials (e.g., SiO_2) have a massive internal surface area that makes them amenable to studies with conventional phonon probes (e.g., Raman, infrared, etc.). The theory involves

treating the system in terms of Bethe lattices which are attached to surface atoms in various ways and describing the potential energy of the atoms in terms of force constant models. Local densities of states along with theoretical Raman, IR and neutron cross sections are being calculated.