model data[4,7] to see if they seem valid there also. To this end we have computed the following (Table I):

$$G(\tau^2, T) = \sum_{m=0}^{\infty} \sum_{n=m+1}^{\infty} g_{m,n} (-\tau^2)^m K^n, \quad (13)$$

where $K = J/kT$ (with J the exchange integral) for square, triangular, simple cubic, bcc, and fcc lattices, to order τ^6 and K^9 or K^{10} for close- or loose-packed lattices, respectively, and (τ^0) and K^8 otherwise. Where comparison is possible, our results agree with those (as corrected) of Opechowski.[8] Except for the coefficient of τ^0 for the two-dimensional lattices, all the coefficients had the expected signs. All the coefficients of the determinants $D(0,1)$ and $D(1,1)$ were positive. Since the coefficient of τ^0 is reduced magnetic susceptibility minus unity and has been extensively studied,[9] there is little doubt that it is positive over the range $T > T_c$ (if any). Consequently, the inequalities which we have proved rigorously for the ferromagnetic Ising model appear to be valid for the ferromagnetic Heisenberg model as well.

Hence we propose that it may be worthwhile to test them experimentally. This test can be made by noting that form (7) implies that

$$(-1)^n \Delta^n G(\tau^2) \geq 0, \quad (14)$$

where Δ is the difference operator with respect to τ^2. That a difference is involved instead of a derivative allows the direct use of experimental data without the difficulty of trying to extract a derivative.

*Work performed under the auspices of the U. S. Atomic Energy Commission.

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INTRINSIC SURFACE STATES IN SEMICONDUCTORS*

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(Reveived 26 February 1968)

Experimentally well established features of semiconductor surface-state distributions are explained in terms of a realistic model calculation.

Calculations reported here for a model crystal surface provide a consistent explanation of the surface-state distributions observed in silicon and germanium, and a simple extension suggests reasons for trends observed in the distributions for III-V and II-VI compounds. These are believed to be the first detailed calculations based on a realistic potential.

A recent survey[1] of measurements on semiconductor-vacuum interfaces indicated two distinct types of behavior. In covalent semiconductors, such as silicon, the densities of surface states and surface atoms are comparable and the Fermi level lies in the lower part of the band gap.

Markedly different are more ionic crystals, which exhibit much lower densities of states. A similar situation appears to exist at semiconductor-metal contacts,[2] though in this case the surface states must be interpreted as tails on the metal wave functions.[3,4]

Calculations of localized states for the (110) face of silicon are reported here. The model is similar to that also suggested by Chaves, Majlis, and Cardona[5] and is described elsewhere.[6] The bulk crystal potential is unaltered up to the surface plane, where it changes abruptly to the vacuum level, determined by work-function measurements. For this model, the calculation sep-

arates into two parts, the first of which is the determination of eigenfunctions of the crystal Hamiltonian with real energies and <u>complex</u> components of momentum $k_\perp$, normal to the surface. Such complex band structures have been determined at several symmetry points of the two-dimensional Brillouin zone using the pseudopotential method.[6] This scheme is known to give a good description of the bulk band structure of many semiconductors[7] and has been adopted in preference to the tight-binding method,[8] which has additional analytical disadvantages.[9] The wave functions for the states in the neighborhood of the semiconductor band gap are dominated by states with wave vectors on the surface of the Jones zone,[10] and basis plane waves have been chosen by symmetry from such wave vectors. For a given $k_\parallel$, the (unchanged) component of the wave vector in the plane of the surface, localized states may now be found by matching these eigenfunctions and their normal derivatives to appropriate vacuum wave functions, i.e., plane-wave states with one component of momentum purely imaginary. The Fourier expansion in $g_\parallel$ is truncated to the leading terms and spin-orbit coupling is neglected, though its inclusion would require no conceptual change.

The two-dimensional Brillouin zone of the (110) face is shown in Fig. 1(a)[11] and the principal results, the surface-state bands in the neighborhood of the gap, are shown in Fig. 1(b). Interpolation between symmetry points utilizes a simplification of the pseudopotential band structure based on the Jones zone. Two basic results emerge:

(1) Two bands of surface states overlap and are degenerate along the line $\bar{Z}$. This degeneracy is a consequence of the glide plane whose translation is in the plane of the surface. The surface states are of the nature described by Shockley[12] and correspond to one state per broken bond. Their appearance as two bands is due to the small size of the surface Brillouin zone relative to the Jones zone.

(2) With one state per surface atom and two atoms per unit cell, one of the above bands should be occupied. For an electrically neutral surface, the Fermi level will lie in the lower half of the gap, in agreement with experiment. The surface levels in this region are sensitive primarily to the splittings $\Gamma_{25}' \rightarrow X_1$, $X_4 \rightarrow X_1$, and $L_3' \rightarrow L_1$. These are essentially the same in silicon and germanium and, as a consequence, similar results may be expected. It should be noted that

some of the surface states are degenerate with volume states with the same $k_\parallel$. Resonant states will result.

The model calculation should provide a good first approximation to the surface-state distribution. As predicted by Heine,[3] the surface-state energies were found to be less sensitive to the precise form of the surface potential than to the phase of the crystal wave functions. In addition, the calculated imaginary components of $k_\perp$ indicate that the states are considerably less localized than the region of expected surface disorder.

The III-V and II-VI compounds may be described by introducing an antisymmetric component into the potential.[7,13] The degeneracy at $\bar{Z}$ will split; a gap in the surface-state distribution will result and will increase with increasing antisymmetry in the potential. This result may be an important factor in an explantion of recent results[2] on CdS_xSe_{1-x}-metal junctions, which seemed to indicate that a continuous transition between the classes mentioned above could occur. With increasing antisymmetry, the occupied and unoccupied bands of surface states would be well separated, with the Fermi level in the region between.

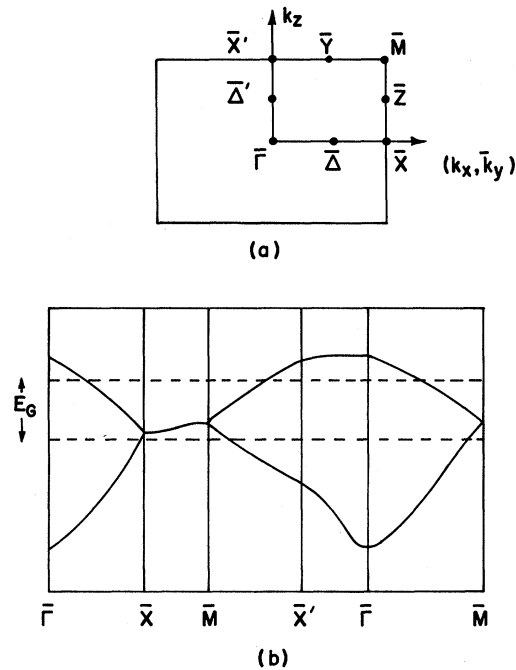The splitting due to the antisymmetric poten-

(a)

(b)

FIG. 1. (a) Two-dimensional Brillouin zone of diamond-structure (110) face. (b) Surface-state energies along different lines of symmetry in zone. The bulk energy gap (1.1 eV) is denoted by E_G.

tial may also explain the absence of intrinsic localized states on ideal oxide-coated silicon surfaces.[14] In tunneling experiments, oxide and vacuum behave quite similarly and it is perhaps paradoxical that they should have such different interface state distributions. In a one-dimensional model, a band gap may be denoted as "S" or "n-S" according to whether or not it gives Shockley states. Matching arguments indicate that no localized states will exist at the boundary between two S-type materials. The absence of intrinsic states on oxides and ionic crystals has formerly been interpreted as resulting from an n-S gap, in which case surface states should exist at an oxide-semiconductor interface. However, the present results and the recent extension of the pseudopotential scheme to MgO[15] suggest that the gap in the oxide may be basically S-type, giving no surface states for oxide-coated silicon or germanium, but with the bands on the oxide-vacuum interface so separated that they are near the edges of the bulk band gap and produce no detectable consequences.

The results described here will not necessarily be identical to those obtained for other crystallographic faces. The (110) face is of particular importance, however, since the semiconducting compounds generally cleave at this face. Calculations on other faces are in progress.

I am indebted to Dr. V. Heine for many stimulating discussions and to Dr. N. W. Ashcroft, Dr. T. K. Bergstresser, and Dr. L. M. Falicov for helpful conversations.

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RECOMBINATION TIME OF QUASIPARTICLES IN SUPERCONDUCTING ALUMINUM

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(Received 13 March 1968)

The quasiparticle recombination time τ_r, has been measured in superconducting aluminum films. The temperature dependence of τ_r at low temperatures was found to be in good agreement with theoretical expectations.

We have measured the recombination time of quasiparticles in superconducting aluminum by a method similar to that of Miller and Dayem (MD).[1] In contrast to their results, but in agreement with theoretical expectations,[2,3] the recombination time τ_r was found to be nearly proportional to $\exp(\Delta/kT)$ at low temperatures. Here, Δ is the (temperature-dependent) energy gap and T the temperature. MD found a much weaker temperature dependence of the form $\exp(\approx 0.3\Delta/kT)$.

As the general experimental technique was adequately described by MD, we give only a brief description here. The measurements were made with a double tunnel junction, shown in Fig. 1(a). Care was taken to prevent direct contact between the indium film and the bottom (400 Å) aluminum film. Excitations (essentially unpaired electrons) are made at a steady rate in both aluminum films by biasing the aluminum-oxide-aluminum tunnel junction (generator) at a bias voltage $V \gtrsim 2\Delta_{Al}/e$, where Δ_{Al} is the energy gap in the aluminum. This increases the quasiparticle density above the thermal equilibrium