sity of Chicago and to Dr. Manuel Cardona and many other members of the staff of RCA Laboratories for stimulating discussions. They are also grateful to Dr. J. C. Phillips and Dr. J. J. Scheer for preprints of their work.

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REFLECTANCE AND PHOTOEMISSION FROM Si†

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We have used the pseudopotential method[1,2] to calculate the energy bands of Si at about 50 000 points throughout the Brillouin zone in a manner similar to that previously reported for Ge.[3] The pseudopotential parameters in rydbergs were chosen to reproduce the energy levels at Γ, X, and L deduced[4] from cyclotron resonance and reflectance data:

$$V_{111} = -0.21, \quad V_{220} = 0.04, \quad V_{311} = 0.08. \qquad (1)$$

The resulting energy bands are shown along the principal symmetry axes in Fig. 1. Neglecting lifetime broadening, the contribution of direct transitions to ϵ_2, the imaginary part of the dielectric constant, is given in terms of the oscillator strength f by

$$\epsilon_2(E_{ij}/h) = \sum_{i,j} f_{ij} N(E_{ij}), \qquad (2)$$

where j labels valence bands, i conduction bands, $E_{ij} = E_i - E_j$, and $N(E)$ is the density of states having energy difference E. We have evaluated ϵ_2 as in reference 3, with the result shown in Fig. 2. (The experimental curve is due to Philipp.[5]) The experimental and theoretical energies at the points of interest shown in Fig. 1 are compared in Ta-

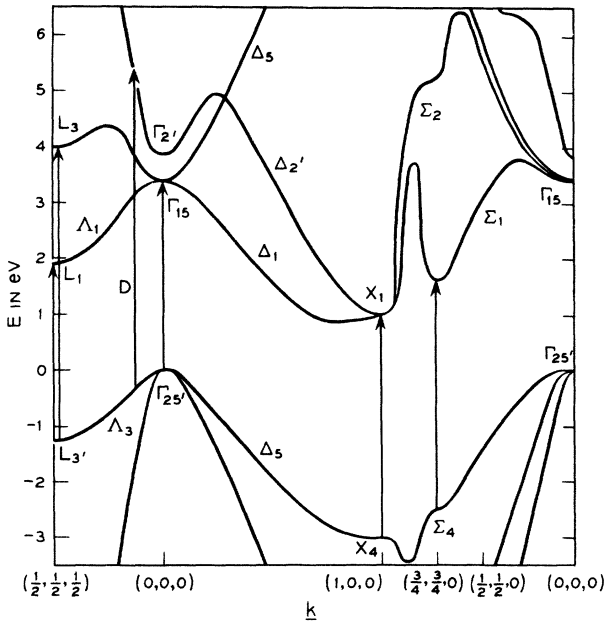

FIG. 1. Energy bands along the principal symmetry axes of the Brillouin zone in Si as calculated using the pseudopotential described in the text. We have marked by arrows the transitions responsible for edges in the reflectance, and have also marked by arrow D the transition associated with special structure in the photoemissivity.

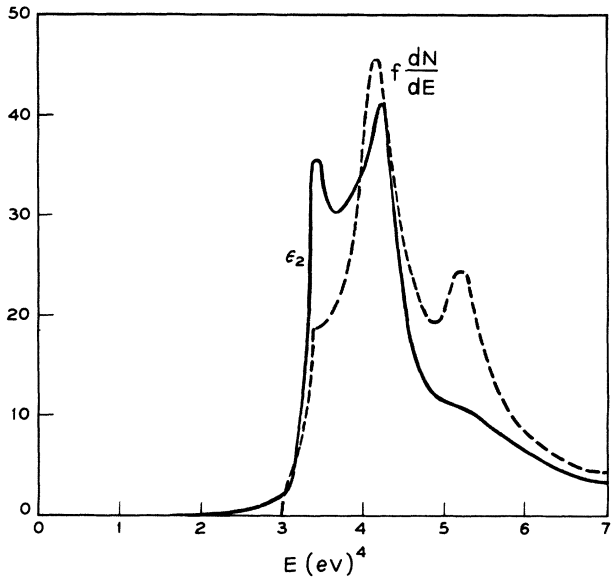

FIG. 2. The imaginary part of the dielectric constant, ϵ_2, as a function of photon energy in Si. The theoretical curve is proportional to $fN(E)$, where f is the oscillator strength and $N(E)$ is the density of valence band→conduction band transitions at a given energy.

ble I. The over-all agreement shown in the table is even better than for Ge, presumably because Si has a small core with occupied s and p levels.[6]

A curious feature of the data unexplained by this calculation is the peak in ϵ_2 at the 3.4-eV edge. Because of the small oscillator strength of exciton transitions, we do not believe that this peak is caused by excitons, as suggested for CdTe.[7] In Ge as well as CdTe similar peaks are probably due to extra structure in $N(E)$ produced by spin-orbit splittings,[8,3] but the Si spin-orbit splitting (~0.03 eV) is too small to account for the peak. It is possible[9] that the peak is a consequence of energy-dependent lifetime broadening $\Gamma(E)$.

The band structure shown in Fig. 1 can now be used to analyze photoemission data which can be conveniently divided into four categories:

(1) Gobeli and Allen's study[10] of threshold emission from atomically clean Si. Kane[11] has shown that the yield near threshold is dominated by a direct process with the excited electron escaping without scattering, together with an indirect tail. The direct and indirect thresholds are at 5.45 and 5.15 eV, so that the direct transition starts from 0.03 eV below the valence band maximum. Kane has also shown that the threshold electrons will have velocity normal to the (111) crystal surface, i.e., have k along the (111) symmetry axis. The transition marked D in Fig. 1 fits Kane's specifications.

(2) The spectral yield from Si covered by one monolayer of Cs.[12] We have calculated the yield, assuming no space-charge band bending at the surface. We have taken vacuum to be W eV above the top of the valence band. We have assumed that emitted electrons have escaped without losing more than 0.1 or 0.2 eV through scattering. The photoemissive yield per photon absorbed is

Table I. Energy differences in eV of principal transitions in Si.

Transition	Experiment	Theory
$\Gamma_{25'}\rightarrow\Delta_1$ (indirect)	1.1	0.9
$\Gamma_{25'}\rightarrow\Gamma_{15}$	3.4	3.4
$L_{3'}\rightarrow L_1$	3.1	3.0
$L_{3'}\rightarrow L_3$	5.4	5.2
$X_4\rightarrow X_1$	4.3	4.0
D in Fig. 1	5.5	5.6

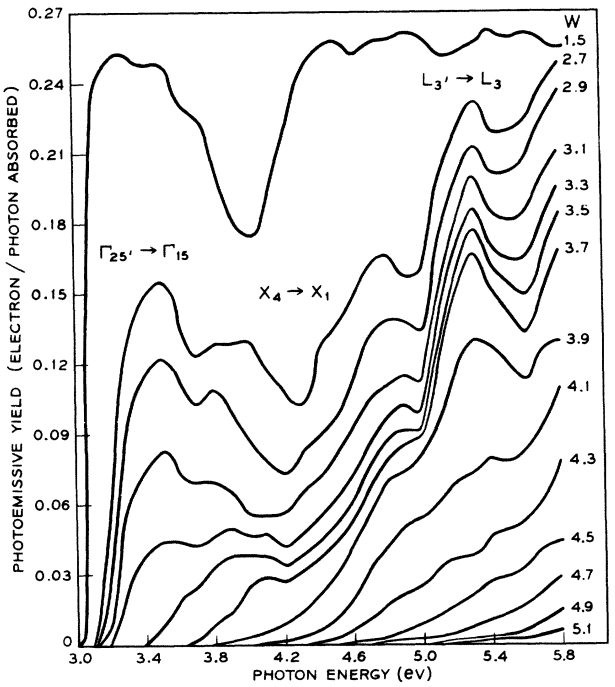

FIG. 3. Photoemissive yield: electrons/absorbed photon as a function of photon energy, with vacuum W eV above the top of the valence band, for a range of values of W corresponding to those experimentally obtainable by covering the Si surface with up to one Cs monolayer. The smallest value of W obtainable in this way is 2.6 eV. If the bulk is sufficiently heavily doped p type, the effective value of W may be 1.5 eV, as suggested by the preceding Letter.

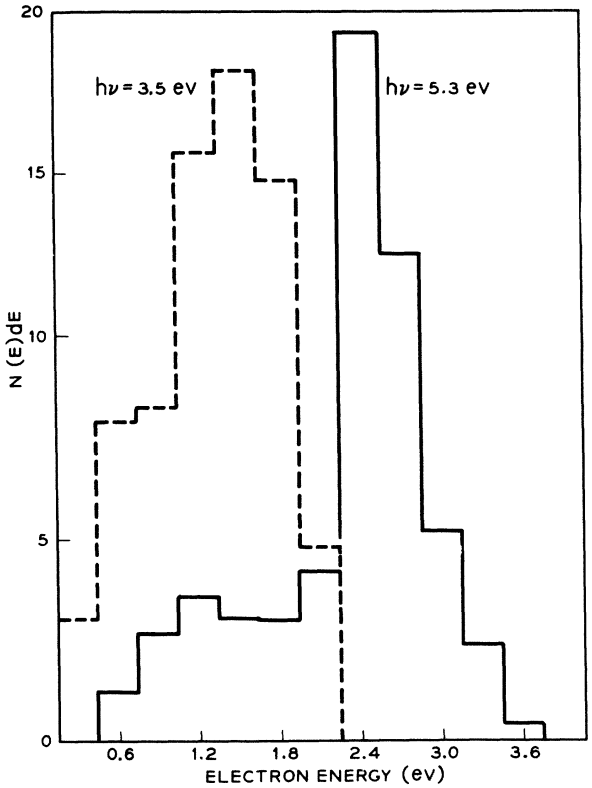

FIG. 4. The energy distribution of electrons emitted from Si for $h\nu = 3.6 \pm 0.1$ eV and 5.3 ± 0.1 eV with $W = 1.5$ eV.

given by

$$Y_W(E) = \sum_{i,j} f_{ij} N(E_{ij}) p(i) \Big/ \sum_{i,j} f_{ij} N(E_{ij}). \qquad (3)$$

Here $p(i)$ is a factor representing the escape probability of electron i, which we have arbitrarily set equal to 0.26 for $E_i > W$ and 0 for $E_i < W$. It appears from Spicer's data and Allen and Gobeli's data that p may depend on surface preparation and may vary with E_i and v_i, but not so drastically as to alter the structure in the yield curve greatly. The principal features of the structure shown in Fig. 3 are the peak at 3.6 eV produced by transitions near $\Gamma_{25'} \rightarrow \Gamma_{15}$, the $X_4 \rightarrow X_1$ dip at 4.3 eV, and the $L_{3'} \rightarrow L_3$ peak at 5.2 eV. Secondary peaks at 3.8 eV and 4.8 eV have been identified as due to transitions near $\Lambda_3 \rightarrow \Lambda_1$ and points in the volume of the Brillouin zone, respectively.

By comparing the heights of the 3.5-eV and 5.5-eV peaks in the yield curves in Fig. 3 for $W = 1.5$ eV and 2.7 eV with the data of the preceding Letter, it appears that the effective W in these data was about 2.1 eV, although W relative to the bulk bands is quoted as 1.4 eV. This difference may be due to having a substantial fraction of the emitted carriers coming from the surface where $W \simeq 2.5$ eV. It may also be due to having an escape probability which is not well approximated by a step function but which increases linearly from 0 at $E_i = W$ to $E_i = W + W'$, and is constant thereafter. In the latter case the preceding data gives $W' \sim 1$ eV.

(3) The spectral yield from Si covered by fractions of a monolayer of Cs studied by Gobeli and Allen.[13] The overall appearance of $Y(E)$ as W varied from 2.7 to 5.1 eV is in good agreement with Fig. 3. For example, the $\Gamma_{25'} \rightarrow \Gamma_{15}$ peak disappears into the background due to uneven coverage at $W =$ about 3.5 eV, as predicted. A careful analysis of these data, which are free of band bending corrections, should yield a value for W'.

(4) The energy distribution $P(E)$ of emitted electrons for $W = 1.5$ eV and several photon energies. Here our sample includes considerably fewer

points, so the energy interval has been made $\Delta E = 0.3$ eV, with the result for $h\nu \simeq 3.5$ eV and 5.3 eV shown in Fig. 4. The two peaks agree well with those observed[12] and confirm the basic assignments $\Gamma_{25'} \rightarrow \Gamma_{15}$ centered at 2.5 eV (more accurately, $\Delta_5 \rightarrow \Delta_1$ and $\Lambda_3 \rightarrow \Lambda_1$) and $L_{3'} \rightarrow L_3$. The width of the low energy peak is determined by the spread in Δ_1 and Λ_1 energy levels. The spread in the $L_{3'} \rightarrow L_3$ peak is also given qualitatively by the variation of Λ_3.

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SCATTERING APPROXIMATION FOR LONG RANGE FORCES*

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Many important contributions in scattering theory have been made through the use of approximations, like the impulse approximation,[1] which treat many-body scattering processes in terms of the individual physical two-body scattering amplitudes. Although these methods have provided powerful tools in the analysis of complicated processes, they have been useful in general for short-range potentials and for large energies and momentum transfers. In this note we describe an approximation which, although considerably different from the impulse approximation, is also formulated in terms of the physical two-body scattering amplitudes. The method is apparently valid for all particle energies and momentum transfers, and requires at least one of the interactions to be long range. Consequently it appears useful in treating a wide variety of elastic and inelastic scattering problems in atomic and nuclear physics. To illustrate and substantiate the theoretical arguments, we show that our methods give rather good agreement with experiments for two different inelastic nuclear processes: the neutron transfer reaction in low-energy ion-ion scattering, and the high-energy (p, d) pickup process.

Before proceeding to the actual approximation we derive an expression that formally obtains the many-body scattering matrix in terms of the two-body amplitudes. For elastic and inelastic (non-rearrangement) scattering a suitable expression can be obtained from a slight modification of existing formulations, such as that of Gell-Mann and Goldberger.[2] Consider the scattering of one particle by another via two potentials U and V; the transition matrix element for this process is given in Eq. (4.4) of reference 2. The total wave function $\psi_a^{(+)}$ defined there can be written in terms of a factorable wave operator acting on an asymptotic