

CALCULATIONS OF TRANSPORT PROPERTIES IN a-Si:H

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Abstract. - We have used the coherent potential approximation to calculate the d.c. conductivity for a model of hydrogenated amorphous silicon. The results show that the mobility of electrons is greater than that of holes. This appears to be related to the strong hydrogen component of the density of states just above the gap.

The incorporation of hydrogen into amorphous Si has been found to change its electronic structure and transport properties drastically. The density of states in the band gap is reduced by several orders of magnitude (1), thereby allowing the "adjustment", by doping (2) with impurities, of the Fermi level E_F which is otherwise pinned near the center of the gap in a-Si. Spectral features related to hydrogenation, such as the removal of states (1) from the gap, the widening of the optical gap (1,3), and the alteration of both the valence (4) and conduction densities of states, have been studied by a variety of theoretical methods (5-8).

The model proposed by two of the authors (6,7) accounts for the data mentioned above as well as showing substantial agreement (7) with the optical absorption data of Cody *et al* (2). In this paper we begin a theoretical study of the transport properties of a-Si:H by calculating the d.c. conductivity for this model system.

The model consists of an effective lattice whose sites have a probability c of being vacant and probability $1-c$ of being occupied by a Si atom. This Si-vacancy alloy provides a model which exhibits many of the properties (6,7) of a-Si. In addition, hydrogen atoms (one, two, three, or four) are incorporated around the vacant site such as to bond with neighboring Si dangling bonds, and the resulting spectral properties reproduce many trends evident in the experimental data on hydrogenation of a-Si. The model is based on a Slater-Koster (SK) Hamiltonian fit (8) to the pseudopotential band structure of Si, and the Coherent Potential Approximation (CPA) is invoked to treat the disorder. The calculational details have been given elsewhere (6,7).

In the present work we treat only the fully hydrogenated case of four hydrogens per vacant Si site. The resulting system shows a very low density of states in the band gap, similar to data on a-Si:H. To evaluate the conductivity σ we begin with the zero frequency Kubo-Greenwood formula

$$\sigma = \frac{2e^2 n}{\pi^2 \Omega m^2} \int dE \left(-\frac{\partial f}{\partial E} \right) \text{Tr} \langle p_x \text{Im} G(E+i\delta) p_x \text{Im} G(E+i\delta) \rangle. \quad (1)$$

where $\langle \dots \rangle$ denotes the configuration average and f is the Fermi function. The evaluation of this expression in a manner consistent

with the CPA has been discussed in detail elsewhere (9). By ignoring the vertex corrections arising from correlations in intermediate scatterings, the Green's functions G can be averaged separately, resulting in the effective medium function \bar{G} . The trace operator Tr in Eq. (1) includes a sum over the Brillouin zone as well as a matrix trace over the basis states, which we have taken as the Bloch sum of s- and p-orbitals which provide the representation for the SK Hamiltonian (8) of silicon. In this basis the momentum (p_x) matrix elements are given by

$$(p_x/m)_{ij} = \hbar^{-1} [H(k+\delta k_x) - H(k)]_{ij} / \delta k_x \quad (2)$$

which we have evaluated numerically by using a finite wavevector displacement δk_x . If a transformation is made to band states which diagonalize H and give eigenvalues E_k , the diagonal elements of p_x/m become the band velocity $dE_k/d(\hbar k)$. However, preliminary evaluation of σ retaining only band-diagonal components of p_x/m has shown that the full matrix nature of this operator must be retained. As opposed to previous CPA evaluations (10) of σ which relied on single band models, we emphasize that the present calculation retains the full multiband character of our model of a-Si:H.

The zone integration of our expression for $\sigma(E)$,

$$\sigma(E) = \frac{2e^2\hbar}{\pi^2\Omega m^2} \sum_k \sum_{ijmn} p_{x,ij} (\text{Im}\bar{G}_{jm}) p_{x,mn} (\text{Im}\bar{G}_{ni}) \quad (3)$$

was done by an analytic tetrahedron approach (11). The irreducible zone (1/48th) was divided into 4000 equal volume tetrahedra (comprising 916 distinct vertices), with the integrand being assumed linear within each tetrahedron. The integration within each tetrahedron can be evaluated analytically, and the result is summed over all 4000 tetrahedra. The same mesh was used to solve for the CPA Green's function \bar{G} and the related density of states $N(E)$. At zero temperature the thermal redistribution ($-\partial f/\partial E$) reduces to a δ -function located at E_F , and Eq. (1) reduces to Eq. (3).

The results for $N(E)$ and $\sigma(E)$ near the gap region are shown in Fig. 1. We find that states very near the top of the valence band at $E \approx -0.5$ eV are only poorly conducting, as the initial increase in $\sigma(E)$ for negative energies occurs below that of $N(E)$. At the top of the gap, however, both $\sigma(E)$ and $N(E)$ show the same "onset" at ~ 0.85 eV. (The energy zero has been set at the bottom of the gap of the reference crystalline Si system (8).)

The comparison of the contribution of electron and hole states to conductivity can be made if we define

$$\sigma(E) = \text{const.} \times \langle p_x^2(E) \rangle N^2(E) \quad (4)$$

which is suggested by the relation $N(E) \propto \text{Im}\bar{G}(E+i\delta)$. The mean square matrix element $\langle p_x^2(E) \rangle$, which describes everything except density of states effects, is 5 to 15 times larger for electron states than for hole states. This difference reflects the character of the states which are involved: hole states derived from bonding combinations of Si-Si and Si-H orbitals, and electron states derived

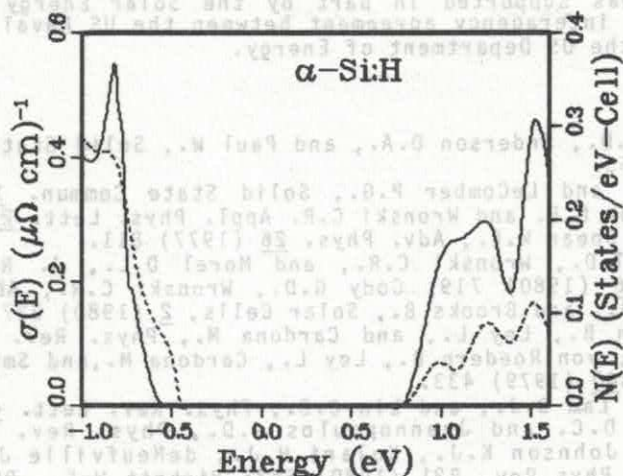


Fig. 1 The zero temperature conductivity $\sigma(E)$ (full line) and density of states $N(E)$ (dashed line) near the gap region for the present model of fully hydrogenated amorphous silicon.

from anti-bonding combinations of these orbitals. Both Si-H combinations are pulled down in energy relative to their Si-Si counterparts, and this is reflected in the ratio $N_H(E)/N_t(E)$ of H local density of states N_H to the total N_t being three times larger for electron states than for hole states ($\sim 7\%$ to 2.5%).

The finite temperature conductivity (ignoring thermal lattice disorder) can be calculated from the relation

$$\sigma(T) = \int dE \left(-\frac{\partial f(E-E_F)}{\partial E} \right) \sigma(E). \quad (5)$$

The results are shown in Fig. 2 for various values of E_F within the gap, corresponding physically to different doping levels. The calculated values of $\log \sigma$ vs. $1/T$ reproduce the approximately linear behavior found in intrinsic and doped samples of a-Si:H (2,12).

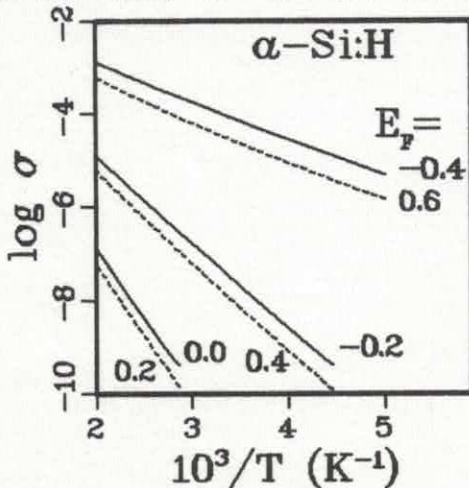


Fig. 2 Logarithm of σ ($\mu\Omega$ cm) $^{-1}$ vs inverse temperature for various placements of E_F , corresponding to different doping levels. Solid lines denote values of E_F in the lower half of the gap ($-0.4, -0.2, 0.0$ eV), while dashed lines are used for values of E_F in the upper part of the gap ($0.2, 0.4, 0.6$ eV).

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