

CALCULATION OF PHYSICAL QUANTITIES IN α -SiH_x

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A simple model of α -SiH_x is studied; its only adjustable parameter is the hydrogen concentration x . By combining the coherent potential approximation with the potential well analogy explicit results are obtained for quantities such as optical absorption, position of mobility edges, mean free path, density of states at the mobility edge, and pre-exponential factor in the dc conductivity. The latter is obtained by neglecting the effects of electron-phonon interaction, which is expected to lead to a strongly temperature-dependent mobility. The theoretical results are in reasonable agreement with experimental data.

1. THE MODEL AND METHODS OF CALCULATION

Over the last few years¹⁻⁴ we have studied a simple model of α -SiH_x. The starting point is a c-Si tight-binding Hamiltonian, H_0 , the matrix elements of which have been obtained by fitting¹ pseudopotential c-Si calculations. Although the fit is good, it can be improved as recent unpublished work of ours indicates. Hydrogen is introduced by randomly replacing Si atoms either by clusters of 4H or by individual H atoms (in the second case it is formally assumed that the Si lattice heals immediately around the H atom).⁴

Our model is definitely not realistic from a structural point of view: it possesses an underline crystallinity and omits the topological disorder; it incorporates no reconstruction (which, however, for high H-concentration may not be so extensive); and it omits many alternative ways of H incorporation. Furthermore, it involves approximations in obtaining the H-H and the Si-H matrix elements.² In spite of these shortcomings and the omission of the off-diagonal disorder in our coherent potential approximation (CPA) calculations,² the results we obtain for the electronic structure are very reasonable. This indicates that the electronic structure of disordered materials is rather insensitive to the structural details, while it depends strongly on local chemical bonding, the size of the unperturbed gap, and the amount of disorder, which can be characterized by a single quantity W , the rms value of the fluctuating potential. The simplifications of our model systematically underestimate W . To compensate for that, one can set the H concentration x

to a higher value than it actually has and/or introduce some additional disorder. We estimated that in order to simulate the real material with $x \approx 15\%$, in our model, x must be around 50% for the 4H cluster case. This indicates that an actual individual H atom is associated with as much disorder as the 4H cluster in our model. For our individual H model good results are obtained if we take x around 30%.

One important advantage of our model is that it contains only one adjustable parameter, namely x . Another advantage is that explicit computations,²⁻⁴ of various quantities of physical interest are possible using the potential well analogy (PWA)⁵ and the CPA. The CPA is used to obtain not only the density of states (DOS) per unit volume, $n(E)$, but the dc and ac conductivity as well, $\sigma^{(o)}(\omega)$. From the $\sigma^{(o)}(\omega)$ one obtains explicit results for the optical absorption α without any assumption about the transition matrix elements. Actually, the CPA implicitly calculates these matrix elements.^{3,4} The CPA dc conductivity $\sigma^{(o)}(0)$ is modified substantially near the band edge due to localization effects. These effects are taken into account by the PWA⁴ method which uses the CPA results as input.

2. RESULTS

Our model reproduces the main qualitative features of $\alpha\text{-SiH}_x$: hydrogen incorporation clears up the gap by passivating the dangling bonds;² hydrogen widens the gap mainly because it reduces the effective ppp interaction and thus shrinks the width of the top peak in the valence band;² the hydrogen-induced peaks in the valence DOS are reproduced fairly well (the 4H model is slightly more successful for the two upper peaks, while the 1H model is definitely better for the third peak).⁴

In Fig. 1 we plot the optical absorption coefficient vs $E = \hbar\omega$. The experimental data are those of Cody.⁶ The solid curve is based on our conductivity CPA calculation,⁴ which implicitly computes the optical transition matrix elements; the dashed line was obtained by convoluting the CPA DOS and assuming that the dipole matrix element $\langle i | x | f \rangle$ ⁴ is on the average energy independent.

Both calculations were done for $x = .3$ by the 1H model (case A). Similar excellent fit for the range 1.7 eV to 3.5 eV is obtained for higher values of x in the 1H model if we introduce additional disorder at the same time so that the total w^2 is doubled (case B). Not only the dependence of α on E is reproduced accurately but its absolute value as well. Thus our conductivity CPA calculation gives values of α which is 16% lower (case A) or 17% higher (case B) than the experimental values. Note also that the assumption of an energy independent average dipole matrix element is obeyed well (in the range 1.7 to

3.5 eV) as witnessed by the almost perfect coincidence of the solid and the dashed curves in Fig. 1.

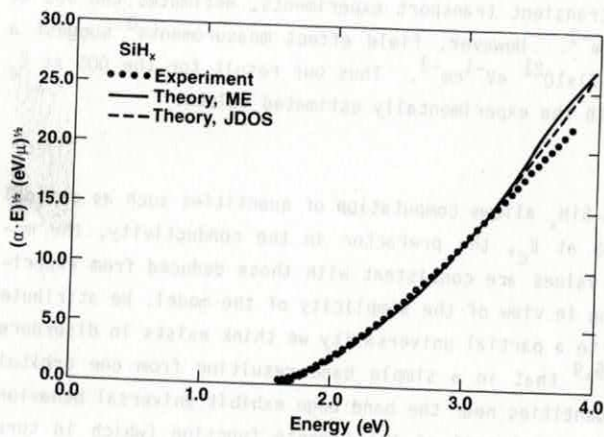


FIGURE 1
Optical absorption coefficient α vs $E = \hbar\omega$. The experimental data are from Ref. 6. The solid line is a full CPA calculation (which includes the determination of the transition matrix elements); the dashed line assumes that the dipole matrix element is energy independent.

Next we present our results for the bottom of the conduction band. (We do not discuss the valence band because it is more complicated both experimentally and as far as the applicability of the PWA is concerned.) The energy dependent CPA dc conductivity (with no phonons included) $\sigma^{(0)}(E)$ was found to be

$$\sigma^{(0)}(E) = C E, \quad (1)$$

where the energy E is measured from the CPA band edge and C is about equal to $5500 (\text{ohm cm eV})^{-1}$ for case A and 2800 for case B. Using the equation $\sigma^{(0)} = e^2 \ell S / 12\pi^3 \hbar$ and the result⁵ that the surface of constant energy $S(E)$ in disordered systems is as in ordered ones but with E measured from the CPA band edge we can obtain the mean free path ℓ . We find $\ell \approx 17\text{Å}$ (case A) or 8Å (case B). Having S and ℓ we can use the equation⁵ $S(E_c)\ell^2(E_c) = 8.96$ to determine the position of the mobility edge E_c relative to the CPA band edge. We find that $E_c \approx 0.0044$ eV (case A) or 0.017 eV (case B). The mobility edge E_c is sensitive to the value of disorder because it is proportional⁵ to w^4 . We are now in a position to obtain the dc conductivity $\sigma(T) = \sigma_0 \exp(-E/kT)$ with the localization effects present⁵ but without phonons. We find that at room temperature the prefactor is $\sigma_0 = 137 (\text{ohm cm})^{-1}$ (case A) or $30 (\text{ohm cm})^{-1}$ (case B). Mott's recent analysis⁷ indicates a value for σ_0 in the range 10 to 70 $(\text{ohm cm})^{-1}$. The mobility at the mobility edge, μ_c , was found to be $28 \text{ cm}^2/\text{V sec}$ (case A) or $11 \text{ cm}^2/\text{V sec}$ (case B). Spear⁸ obtained values in the range 10 to $24 \text{ cm}^2/\text{V sec}$ in good agreement with our present results. The DOS per unit volume calculated from our model is $AE^{1/2}$ for $E_c < E < 0.3$. For lower values of E exponential tail states appear, while for higher values the energy depend-

ence turns to linear in E . The constant A is $7.5 \times 10^{21} \text{ eV}^{-3/2} \text{ cm}^{-3}$. Thus the DOS at the mobility edge is $5 \times 10^{20} \text{ eV}^{-1} \text{ cm}^{-3}$ (case A) or $10^{21} \text{ eV}^{-1} \text{ cm}^{-3}$ (case B). Spear⁸, on the basis of transient transport experiments, estimates the DOS at E_c as being $5 \times 10^{20} \text{ eV}^{-1} \text{ cm}^{-3}$. However, field effect measurements⁸ suggest a larger C value around $(1-2) \times 10^{21} \text{ eV}^{-1} \text{ cm}^{-3}$. Thus our result for the DOS at E_c seems to be consistent with the experimentally estimated values.

3. CONCLUSIONS

Our simple model for $\alpha\text{-SiH}_x$ allows computation of quantities such as optical absorption coefficient, DOS at E_c , the prefactor in the conductivity, the mobility at E_c , etc. Our values are consistent with those deduced from experiments. This is surprising in view of the simplicity of the model. We attribute the success of our model to a partial universality we think exists in disordered systems. We have shown^{5,9} that in a simple band resulting from one orbital per unit cell, several quantities near the band edge exhibit universal behavior, while others depend on the real part of the Green's function (which in turn depends on the details of the band). Although the extent of this universality in a situation of two bands with more orbitals per site, as in $\alpha\text{-SiH}_x$, is not fully understood, the success of the present model suggests that universality still exists and that it allows correct results to be extracted from simplified models which retain only the truly significant features of realistic systems.

REFERENCES

1. D.A. Papaconstantopoulos and E.N. Economou, Phys. Rev. B22, 2903 (1980).
2. D.A. Papaconstantopoulos and E.N. Economou, Phys. Rev. B24, 7233 (1981).
3. W.E. Pickett, D.A. Papaconstantopoulos, and E.N. Economou, Phys. Rev. 28, 2232 (1983).
4. A.D. Zdetsis, E.N. Economou, D.A. Papaconstantopoulos and N. Flytzanis, Phys. Rev. B31, 2410 (1985).
5. E.N. Economou, C.M. Soukoulis, and A.D. Zdetsis, Phys. Rev. B30, 1686 (1984); B31, 6172 (1985).
6. G.D. Cody in "Semiconductors and Semimetals", Vol. 21 B, J. Pankove, ed., Academic Press (1984), (Fig. 14) and private communication.
7. N.F. Mott, Phil. Mag. B51, 19 (1985).
8. W.E. Spear, J. of Non. Cryst. Sol. 59-60, 1 (1983).
9. M.H. Cohen, E.N. Economou, C.M. Soukoulis, submitted for publication.