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Optical absorption in amorphous semiconductors

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We use the joint density-of-states function to study the optical-absorption spectrum of amorphous semiconductors. To determine the overall joint density of states, we average a local joint density of states over spatially correlated Gaussian distributions of conduction-band and valence-band potential fluctuations. Our results span the transition from below to above the energy gap and both analytical and numerical results are obtained. Spatial correlations are found to play a dramatic role in influencing the shape of the optical-absorption spectrum. We apply this formalism to the case of hydrogenated amorphous silicon and several other amorphous semiconductors of interest, and find that our results are consistent with those of experiment.

Optical absorption in amorphous semiconductors has been the subject of extensive study.[1-4] While the subgap absorption features have been well characterized by such analyses, the transition in the functional form of the optical-absorption coefficient $\alpha(\hbar\omega)$, from below to above the gap, is still not well understood.[5] In order to help address this deficiency, in a recent paper[6] we presented a semiclassical density-of-states (DOS) analysis of amorphous semiconductors. This analysis, cast within an effective-mass framework, determined the overall conduction- and valence-band DOS functions by averaging local DOS functions over independent distributions of conduction- and valence-band potential fluctuations. With these DOS functions determined, we then calculated, numerically, the joint density-of-states (JDOS) function $J(\hbar\omega)$, the functional properties of $\alpha(\hbar\omega)$ being essentially dominated by those of $J(\hbar\omega)$.[7,8]

In this paper, we perform a more general optical-absorption analysis. We evaluate the JDOS function by averaging a local JDOS function over the distribution of conduction- and valence-band potential fluctuations, i.e., $J(\hbar\omega)=\langle J^{\mathrm{loc}}(\hbar\omega)\rangle$, where the local JDOS function

$$J^{\mathrm{loc}}(\hbar\omega)=\int N_c^{\mathrm{loc}}(E)N_v^{\mathrm{loc}}(E-\hbar\omega)dE \ . \tag{1}$$

$N_c^{\mathrm{loc}}(E)$ and $N_v^{\mathrm{loc}}(E)$ denote the local conduction- and valence-band DOS functions, respectively. This analysis allows us to examine the effect of spatial correlation between the fluctuations in the individual bands. For the special case of independent conduction- and valence-band potential fluctuations, this reduces to the standard expression for the JDOS function found in the literature,[7,8] i.e.,

$$J(\hbar\omega)=\int N_c(E)N_v(E-\hbar\omega)dE \ , \tag{2}$$

where $N_c(E)$ and $N_v(E)$ denote the conduction- and valence-band DOS functions, respectively.

Following Ref. 6, in a local region about $\mathbf{R}$, we assume that

$$N_c^{\mathrm{loc}}(E)=\frac{\sqrt{2}m_c^{*3/2}}{\pi^2\hbar^3}\sqrt{E-V_c(\mathbf{R})} \tag{3}$$

and

$$N_v^{\mathrm{loc}}(E)=\frac{\sqrt{2}m_v^{*3/2}}{\pi^2\hbar^3}\sqrt{V_v(\mathbf{R})-E} \ , \tag{4}$$

where m_c^* and m_v^* denote the effective mass of electrons in the conduction band and holes in the valence band, respectively, and $V_c(\mathbf{R})$ and $V_v(\mathbf{R})$ represent the corresponding potential profiles. Thus, the local JDOS function becomes

$$J^{\mathrm{loc}}(\hbar\omega)=\begin{cases}\dfrac{\sqrt{2}m_c^{*3/2}}{\pi^2\hbar^3}\dfrac{\sqrt{2}m_v^{*3/2}}{\pi^2\hbar^3}\dfrac{\pi}{8}[\hbar\omega-E_g(\mathbf{R})]^2 \ , & \hbar\omega\ge E_g(\mathbf{R})\\ 0 \ , \quad \hbar\omega<E_g(\mathbf{R}) \ , & \end{cases} \tag{5}$$

where $E_g(\mathbf{R})$ denotes the local energy gap, $E_g(\mathbf{R})\equiv V_c(\mathbf{R})-V_v(\mathbf{R})$. To determine the overall JDOS function, we average Eq. (5) over the distribution of energy-gap fluctuations, to obtain

$$J(\hbar\omega)=\frac{\sqrt{2}m_c^{*3/2}}{\pi^2\hbar^3}\frac{\sqrt{2}m_v^{*3/2}}{\pi^2\hbar^3}\mathcal{J}(\hbar\omega) \ , \tag{6}$$

where the normalized JDOS function

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$$\mathcal{J}(\hbar\omega) \equiv \frac{\pi}{8}\int_{-\infty}^{\hbar\omega}(\hbar\omega - z)^2 f_{E_g}(z)dz \ . \qquad (7)$$

$f_{E_g}(z)\Delta z$ denotes the probability that $E_g(\mathbf{R})$ is between $[z, z+\Delta z]$.

We perform our analysis under the assumption of spatially correlated Gaussian distributions of conduction- and valence-band potential fluctuations. Letting η_c and η_v denote the mean potential associated with $V_c(\mathbf{R})$ and $V_v(\mathbf{R})$, respectively, σ_c and σ_v being the corresponding standard deviations, we find that

$$f_{E_g}(z) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(z - E_{g_0})^2}{2\sigma^2}\right] , \qquad (8)$$

where the mean energy gap $E_{g_0} \equiv \eta_c - \eta_v$, and the energy-gap variance

$$\sigma^2 \equiv \sigma_c^2 + \sigma_v^2 - 2\rho\sigma_c\sigma_v \ ; \qquad (9)$$

ρ represents the correlation between $V_c(\mathbf{R})$ and $V_v(\mathbf{R})$, this coefficient ranging between 1 and -1.[9] We note that if the fluctuations in $V_c(\mathbf{R})$ and $V_v(\mathbf{R})$ tend to be parallel ($\rho \simeq 1$), as in the case for electrostatic potential fluctuations, then σ is smaller; if the fluctuations tend to be antiparallel ($\rho \simeq -1$), as in response to the strain associated with topological disorder, then σ is larger. For the special case of independent conduction- and valence-band potential fluctuations, $\rho = 0$, and $\sigma^2 = \sigma_c^2 + \sigma_v^2$.

We now determine the form of the normalized JDOS function $\mathcal{J}(\hbar\omega)$. From Eqs. (7) and (8), we obtain

$$\mathcal{J}(\hbar\omega) = \frac{\pi}{8}\sigma^2\,\Theta\left[\frac{\hbar\omega - E_{g_0}}{\sigma}\right] , \qquad (10)$$

where

$$\Theta(z) \equiv \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{z}(z - x)^2\exp\left[-\frac{x^2}{2}\right]dx \ . \qquad (11)$$

We note that while E_{g_0} determines the positioning of the JDOS function, σ dictates the spread. Asymptotic analysis shows that, for energies well above E_{g_0},

$$\mathcal{J}(\hbar\omega) \to \frac{\pi}{8}[(\hbar\omega - E_{g_0})^2 + \sigma^2] , \qquad (12)$$

while, for energies well below E_{g_0},

$$\mathcal{J}(\hbar\omega) \sim \exp\left[-\frac{|\hbar\omega - E_{g_0}|^2}{2\sigma^2}\right] . \qquad (13)$$

To study how spatial correlations shape the JDOS function, in Fig. 1 we plot the functional dependence of $\mathcal{J}(\hbar\omega)$ for ρ varying between -1 and 1, σ_c and σ_v both being set at 150 meV. We note that the breadth of the subgap absorption tail is a strong function of ρ. If the potential fluctuations in the conduction and valence bands are completely parallel ($\rho = 1$), then there will be no variation in the local energy gap, and the optical-absorption spectrum will terminate abruptly at the mean energy gap E_{g_0}. In contrast, for completely antiparallel potential fluctuations ($\rho = -1$), a broad subgap absorption tail is observed.

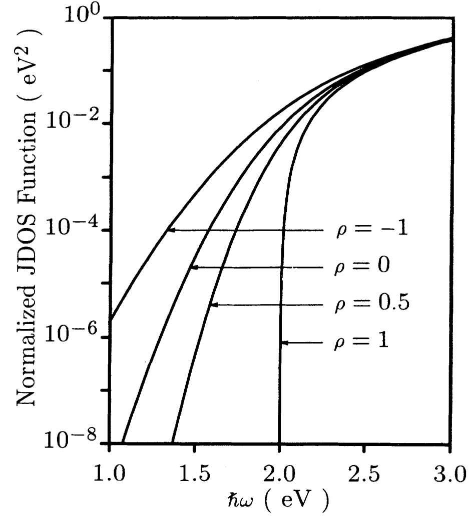

FIG. 1. The normalized JDOS function $\mathcal{J}(\hbar\omega)$ with variations in the correlation coefficient ρ. E_{g_0} is set to 2 eV, and σ_c and σ_v are both set to 150 meV, for all cases.

We now apply this formalism. Initially, we focus on the determination of σ and E_{g_0}, the determination of ρ being dealt with below. Optical absorption in three different amorphous semiconductors is considered: (1) hydrogenated amorphous silicon (*a*-Si:H); (2) amorphous

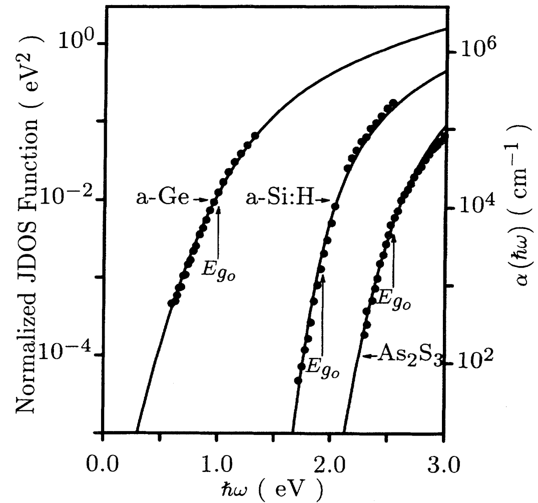

FIG. 2. Optical absorption for three different amorphous semiconductors. Theoretical curves are depicted by solid lines. Experimental data points are depicted by solid points. The experimental data for *a*-Si:H, *a*-Ge, and *a*-As_2S_3 is from Cody (Ref. 10), Theye (Ref. 11), and Street *et al.* (Ref. 12), respectively. For the *a*-Si:H data of Cody (Ref. 10), $\alpha(\hbar\omega) = 3.96 \times 10^6 \mathcal{J}(\hbar\omega)$, where $\mathcal{J}(\hbar\omega)$ is in units of eV^2 and $\alpha(\hbar\omega)$ is in units of cm^{-1}. For the *a*-Ge data of Theye (Ref. 11) and the *a*-As_2S_3 data of Street *et al.* (Ref. 12), $\alpha(\hbar\omega) = 1.25 \times 10^6 \mathcal{J}(\hbar\omega)$. The $\alpha(\hbar\omega)$ scale shown in the above figure corresponds to the latter normalization.

germanium (a-Ge), of similar structure to a-Si:H; and (3) amorphous arsenic trisulphide (a-As_2S_3), a chalcogenide glass. In Fig. 2, optical-absorption data for a-Si:H,[10] a-Ge,[11] and a-As_2S_3 (Ref. 12) are plotted; these results have been scaled by a constant factor to facilitate a comparison with $\mathcal{J}(\hbar\omega)$, the scaling between $\alpha(\hbar\omega)$ and $\mathcal{J}(\hbar\omega)$ being consistent with that of Jackson *et al.*[8] Alongside, we plot our theoretical result for the following parameter selections: for a-Si:H, $\sigma=162$ meV and $E_{g_0}=1.93$ eV; for a-Ge, $\sigma=250$ meV and $E_{g_0}=1.00$ eV; and for a-As_2S_3, $\sigma=165$ meV and $E_{g_0}=2.55$ eV. We note that, in all cases, the agreement between theory and experiment is excellent, both below and above the energy gap.

We now estimate ρ for the case of high-quality a-Si:H. Analysis of time-of-flight data suggests that for high-quality a-Si:H σ_c is between 90 and 100 meV and σ_v is between 130 and 145 meV.[6] The present optical-absorption analysis, applied to a similar high-quality a-Si:H, suggests that σ is 162 meV. From Eq. (9), it follows that spatial correlation effects play a small role in shaping the optical-absorption spectrum of high-quality a-Si:H, i.e., $\rho \simeq 0$.

In conclusion, we have presented an elementary semiclassical optical-absorption analysis of amorphous semiconductors which successfully predicts some of the basic qualitative and quantitative features of the joint density-of-states function. This analysis spans the transition from below to above the gap, and adequately characterizes experimental optical-absorption data over many orders of magnitude. Furthermore, the present approach readily takes into account the possibility of a spatial correlation between the conduction- and valence-band potential fluctuations.

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