Active and Passive Elec. Comp., 1993, Vol. 16, pp. 65–68
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SOME NEW RESULTS ON VIBRATIONAL PROPERTIES OF AMORPHOUS GROUP IV SEMICONDUCTORS

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(Received April 2, 1993; in final form May 5, 1993)

For neutron scattering, an interesting formula is derived from the coherent one-phonon dynamic structure factor. In this derivation, phonon density of states is involved; this density is related to spectra due to structural disorder, which is investigated. Our considerations refer to amorphous Group IV semiconductors.

1. INTRODUCTION

Inelastic neutron scattering has been employed extensively in order to analyze vibrational spectra of a large number of amorphous semiconductors. In the following, we shall study one-phonon dynamic structure factor and phonon density of states. Calculations related to this density are relevant in the context of inelastic neutron scattering for amorphous Ge and Si.

We shall consider a density of states corresponding to the inelastic scattering spectrum of a one-component amorphous quasi-harmonic solid. On the other hand, we can claim that reliable measurements of phonon density of states for Group IV semiconductors were performed by various workers [1, 2].

2. THEORY

Following Alben [3], the coherent one-phonon dynamic structure factor for a model structure is given by [4]:

$$S(\vec{q}, E) = (\hbar/m\omega)\left(v + \frac{1}{2}\right) \sum_{n} \left\{ \left| \vec{q}\cdot\sum_{\alpha} [\vec{u}_{n\alpha} \exp(i\vec{q}\cdot\vec{r}_{\alpha})] \right|^2 \delta(E - E_n) \right.$$
$$\left. \times \exp(-2W) \right\} \qquad (i = \sqrt{-1}) \quad (1)$$

where m is the mass, which is the same for all sites; $\hbar$ is the modified Planck constant; ω is the angular frequency; v is the vibrational quantum number; $\vec{q}$ is transferred momentum; $\vec{u}_{n\alpha}$ is the normalized eigenvector corresponding to displacement of the α^{th} atom and referred to n^{th} mode; the vectors $\vec{r}_\alpha$ are the equilibrium positions; δ means Dirac function; E is energy; E_n is the energy of the n^{th} mode; and W is here the site-independent Debye-Waller factor.

Now we introduce [3]:

$$S'(\vec{q}, E) = S(\vec{q}, E) \Big/ \left[\frac{\hbar}{m\omega}\left(v + \frac{1}{2}\right)\frac{1}{3} q^2 \exp(-2W)\right] \tag{2}$$

where q is the modulus of $\vec{q}$.

From (1) and (2) it is deduced:

$$|S'(\vec{q}, E)| = S'(\vec{q}, E) \leqslant 3 \sum_n^N \delta(E - E_n) \sum_\alpha^N |\vec{u}_{n\alpha}|^2 \tag{3}$$

On the other hand, it is well-known that $S'(\vec{q}, E) \equiv g(E)$ in the incoherent limit of q (large q) [3]; g(E) is the phonon density of states. Therefore we can establish:

$$g(E) = 3 \sum_n^N \delta(E - E_n) \sum_\alpha^N |\vec{u}_{n\alpha}|^2 \tag{4}$$

We also can write [5]:

$$g(\omega) = \frac{1}{3} q^2 N^{-1} \exp(-2W) \sum_n^N \delta(\omega - \omega_n) \tag{5}$$

By changing E with ω in (4) ($\hbar = 1$ in atomic units), we have:

$$\int_\Omega g(\omega)\, d\omega = 3 \sum_{n,\alpha}^N |\vec{u}_{n\alpha}|^2 \tag{6}$$

by taking into account [6, 7]:

$$\int_\Omega \delta(\omega - \omega_n)\, d\omega = 1$$

where Ω is the ω-domain and ω_n is the vibrational eigenfrequency of the n^{th} normal mode of the solid.

From (5) we obtain:

$$\int_\Omega g(\omega)\, d\omega = (q^2/3) \exp(-2W) \tag{7}$$

since $\sum_{n=1}^N 1 = N$

Finally from expressions (6) and (7) we get:

$$\sum_{n,\alpha}^{N} |\vec{u}_{n\alpha}|^2 = (q/3)^2 \exp(-2W) \tag{8}$$

Formula (8) involves vibrational eigenvectors and refers to large q. Next we shall consider structural disorder in amorphous Group IV semiconductors; in the context of tetrahedrally coordinated amorphous semiconductors, the first-order infrared spectrum due to structural disorder can be expressed as follows [8, 9, 10]:

$$\xi_2^{(s)}(\omega) = \omega^{-2}|\mu(\omega)|^2 g(\omega) \tag{9}$$

where $\mu(\omega)$ is the dipole-moment matrix element in the frequency domain.

Now it is interesting to evaluate the important quantity $\int_\Omega \omega\xi_2^{(s)}(\omega)\, d\omega$; we have:

$$\int_\Omega \omega\xi_2^{(s)}(\omega)\, d\omega = 3 \sum_{n}^{N} \sum_{\alpha}^{N} |\vec{u}_{n\alpha}|^2 \int_\Omega \omega^{-1}|\mu(\omega)|^2\, \delta(\omega - \omega_n)\, d\omega \tag{10}$$

(see eq. (4))

We get as final result (see refs. [6, 7]):

$$\int_\Omega \omega\xi_2^{(s)}(\omega)\, d\omega = 3 \sum_{n}^{N} \omega_n^{-1}|\mu(\omega_n)|^2 \sum_{\alpha}^{N} |\vec{u}_{n\alpha}|^2 \tag{11}$$

3. DISCUSSION

At large q, coherent processes are not relevant. In fact, eqs. (4) and (11) refer to this situation. It is well-known that inelastic neutron scattering at fixed and large q makes possible the direct measurement of the phonon density of states. This density can be obtained theoretically by means of eq. (5) or by using the expression $g(\omega) = 3\,\Sigma_n^N\, \delta(\omega - \omega_n)\, \Sigma_\alpha^N\, |\vec{u}_{n\alpha}|^2$ (see eq. (4)). In addition, eq. (8) represents a result derived from the conjunction of the previous expression and eq. (5). Equation (8) can be expressed as: $(\Sigma_{n,\alpha}^N\, |\vec{u}_{n\alpha}|^2)^{1/2} = \frac{1}{3}q \times \exp(-W)$; this expression is interesting from the point-of-view of mathematical physics since its left-hand side represents a norm associated with a certain Hilbert space equipped with the scalar product $\langle \vec{u}_{n\alpha}, \vec{w}_{n\alpha} \rangle = \Sigma_{n,\alpha}^N\, (\vec{u}_{n\alpha} \cdot \vec{w}_{n\alpha})$, where the dot means usual scalar product. Moreover, we recall the physical sense of $S'(\vec{q}, E)$; this quantity represents energy loss spectra.

Finally, we recall also the importance of eq. (11). The left-hand side of this is the structural-disorder contribution to the sum rule $\int_\Omega \omega\xi_2(\omega)\, d\omega$.

APPENDIX

In fig. A1 we can compare the energy loss spectrum $S'(\vec{q}, E)$ with $g(E)$ for $q = 17.0$ Å^{-1} and amorphous Ge, by using a periodic network model (see ref. [3]). In

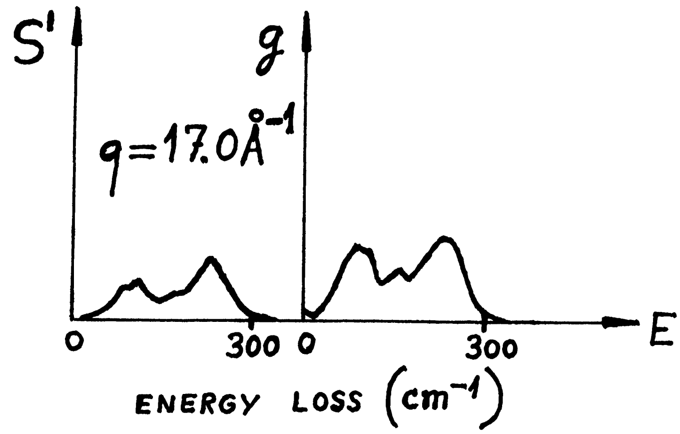

FIGURE A1 Plots of S′ and g for amorphous Ge with respect to a periodic network model.

addition, it is interesting to note the comparison between the plot of g(E) and eq. (4).

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