FIRST-ORDER OPTICAL PHONON PROCESSES IN AMORPHOUS CLUSTERS

M.A. GRADO CAFFARO, consultant (Madrid, Spain) and
M. GRADO CAFFARO, consultant (Madrid, Spain)

C./Julio Palacios, 11, 9ºB, 28029—Madrid (Spain)

Optical absorption in the far infrared range for amorphous GaAs, SiC and Ge is investigated. Small clusters in the context of dynamical disorder are considered. Average values of the absorption contributions due to both dynamical and structural disorders are introduced. In particular, an equation for the spectrum due to dynamical disorder in amorphous SiC is presented.

I. INTRODUCTION

In the following, we shall refer to silicon carbide, germanium and III-V semiconductors in their amorphous state. Certain considerations on the above materials are also valid for other amorphous semiconductors. We shall study both dynamical and structural disorders by considering average values of optical absorption in the far infrared range.

Recently, both theoretical and experimental work on amorphous SiC has been developed by using a conventional methodology. We shall analyse SiC behavior in its amorphous state in a special way so that comparison of this behavior with the optical properties of Ge, Si and GaAs is feasible.

II. THEORETICAL FORMULATION

First, let us consider small clusters in amorphous GaAs. M.A. Grado and M. Grado have obtained recently the following expression for dynamical disorder:[1]

$$\xi_2^{(d)}(\omega) \approx ar_o \left(1 - \frac{1}{3} br_o^2 \right) (\xi_o - \xi_\infty) \omega_{TO(c)} \gamma_c^{-1} \omega \tag{1}$$

To derive eq. (1) a small cluster is assumed, so that the "length" of the cluster, r_o, is small. Moreover, we have considered $\omega_{TO} = \omega$; ω_{TO} stands for the angular frequency of the transversal optical mode and we have supposed that ω_{TO} does not depend approximately on r (distance) in the cluster considered. In eq. (1) a and b are constants (a > 0; b > 0), ξ_o is the value of the imaginary part of the static

dielectric constant, ξ_∞ is the value of the imaginary part of the high-frequency dielectric constant, $\omega_{TO(c)}$ is the angular frequency of the transversal optical mode in the crystalline state, and γ_c is a damping factor.

On the other hand, the spectrum due to structural disorder is given by[1-3].

$$\xi_2^{(s)}(\omega) \approx Kg(\omega) \tag{2}$$

where K is a constant and $g(\omega)$ is the phonon density of states. Eq. (2) is valid for the far infrared range. Hereafter, we shall consider this range only.

Then, total spectrum is given by

$$\xi_2(\omega) \approx Kg(\omega) + K'\omega \tag{3}$$

where K' is a constant namely:

$$K' = ar_0 \left(1 - \frac{1}{3} br_0^2\right) (\xi_0 - \xi_\infty)\gamma_c^{-1}\omega_{TO(c)}$$

and $\xi_2(\omega)$ is given by[1,4,5]

$$\xi_2(\omega) \approx K \int_0^{\hbar\omega} g(E)g(\hbar\omega - E) \, dE \tag{4}$$

for $\hbar\omega > 2E_c$; $\hbar$ is the modified Planck constant ($\hbar \equiv h/2\pi$), E stands for electronic energy, and E_c is the energy at the conduction band edge. Eq. (4) can be expressed as a convolution, namely:

$$\xi_2(\omega) \approx K[g(\omega)] * [g(\omega)] \tag{5}$$

Hereafter, we will consider the case in which $\hbar\omega > 2E_c$ exclusively. By applying Laplace transform in eq. (5) we get:

$$g(\omega) = K^{-1/2} \pounds^{-1}\{\{\pounds[\xi_2(\omega)]\}^{1/2}\} \tag{6}$$

where £ stands for the Laplace transform operator.

Next we will take average values in both sides of eq. (3) by taking into account eq. (4). We get

$$\int_0^\Omega d\omega \int_0^\omega g(E)g(\omega - E) \, dE \approx \int_0^\Omega g(\omega) \, d\omega + \frac{1}{2}\frac{K'}{K}\Omega^2 \tag{7}$$

where Ω is the maximum angular frequency in the far infrared range; for convenience, we have taken $\hbar = 1$ (atomic units). Eq. (7) is an interesting relationship in terms of the phonon density of states. From this equation we consider the following average values:

$$\langle\xi_2^{(d)}(\omega)\rangle = \frac{1}{2}K'\Omega \tag{8}$$

$$\langle \xi_2^{(s)}(\omega) \rangle = K\Omega^{-1} \int_0^{\Omega} g(\omega) \, d\omega \tag{9}$$

In amorphous SiC, dynamical disorder corresponds to the following absorption spectrum[2]

$$\xi_2^{(d)}(\omega) = a(\xi_o - \xi_\infty)\gamma_c \left\{ \int_R (\exp(-br^2)) \right.$$

$$\left[\frac{\omega_{TO}^3}{\omega_{TO(c)}^2(\omega_{TO}^2 - \omega^2)^2 + (\gamma_c\omega\omega_{TO}^{1/2})^2} + \frac{\omega_{LO}^3}{\omega_{LO(c)}^2(\omega_{LO}^2 - \omega^2)^2 + (\gamma_c\omega\omega_{LO}^{1/2})^2} \right] dr \left. \right\} \omega \tag{10}$$

where ω_{LO} is the angular frequency corresponding to the longitudinal optical mode; both ω_{TO} and ω_{LO} depend on distance, r, R being the r-domain.

Finally we shall consider very briefly amorphous Ge. It is well known that for this material we can assume $\xi_2(\omega) = \xi_2^{(s)}(\omega)$ (see ref. [2]). Then by combining eq. (2) with eq. (5) it is deduced: $g(\omega) = \delta(\omega)$ (Dirac delta). In fig. 1 (see ref. [6]) we can observe the variation of $\omega\xi_2$ as a function of the wave-number for amorphous Ge. From our theoretical considerations, we have $\omega\xi_2(\omega) = K\omega\delta(\omega)$. This result agrees with fig. 1 in the range 0–100 cm^{-1}.
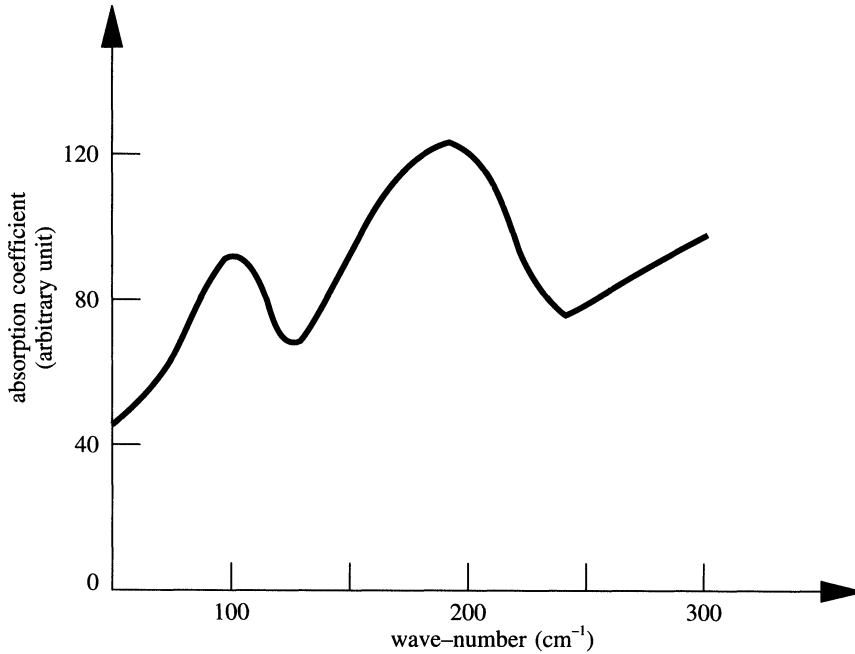

FIGURE 1 Experimental plot of the absorption coefficient as a function of the wave-number for amorphous Ge (after ref. [6]).

III. CONCLUSION

Phonon density of states plays an important role in the context of amorphous solids. In particular, the relation between this density in amorphous III-V compounds and the no verification of the wave-vector conservation has been studied in various research works (see, for example, [6] [7]). This problem has been also considered in amorphous SiC. This material has been investigated recently by several workers (see, for instance, ref. [8]) but the physical mechanisms associated with ω_{TO}, ω_{LO} and dynamical disorder remain unclear. Finally, with respect to amorphous GaAs, eq. (7) is an important result.

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