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A STUDY ON THE TRANSVERSAL OPTICAL MODE IN AMORPHOUS GALLIUM ARSENIDE

M. A. GRADO-CAFFARO* and M. GRADO-CAFFARO

Scientific Consultants, C/Julio Palacios, 11, 9-B, 28029-Madrid, Spain

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Contributions to the far-infrared spectrum corresponding to both dynamical and structural disorders in a-GaAs are examined when frequency coincides with the transversal optical mode. Under these circumstances, dipole moment matrix element is discussed.

Keywords: Far-infrared spectrum; a-GaAs; transversal optical mode; dipole moment matrix element

1. INTRODUCTION

Transverse optical mode in amorphous III-V semiconductors presents a great relevance with respect to the far-infrared spectrum corresponding to dynamical disorder; in this context, the frequency associated with this mode is a function of distance. Coincidence of this frequency with the generic frequency has been examined in Ref. [1]. On the other hand, this coincidence has a great importance in the variations of the dipole moment matrix element [2]. Really these subjects are very interesting and the main problems associated with them are still unsolved in a major part at least from the point of view of theory. In the following, we shall try to clarify some of these problems for amorphous gallium arsenide.

*Corresponding author.

2. THEORY

First of all, consider the expression of the far-infrared spectrum corresponding to dynamical disorder for a-GaAs namely [1, 2, 3, 4]:

$$\varepsilon_2^{(d)}(\omega) = a(\varepsilon_o - \varepsilon_\infty)\gamma_c \omega_{TO(c)}\omega \int_o^R \frac{\omega_{TO}^3(r)\exp(-br^2)dr}{\omega_{TO(c)}^2(\omega_{TO}^2(r) - \omega^2)^2 + \gamma_c^2\omega^2\omega_{TO}^2(r)} \quad (1)$$

where ω denotes angular frequency, a and b are positive constants, TO stands for transversal optical mode, (c) denotes crystalline state, γ_c is the damping factor and r is distance (we consider a one-dimensional model).

Next we will assume that, although ω_{TO} depends upon distance, the region of dynamical disorder is sufficiently small so that ω_{TO} can be regarded as approximately constant; structural disorder will be assumed as a considerable disorder so that the total contribution to disorder may be conceived as appreciable. In fact, this situation takes place for example, in a-Ge as a dynamically and structurally disordered material. Under the above conditions for a-GaAs and by taking into account that the dipole moment matrix element is considerably larger for $\omega = \omega_{TO}$ than that for the other frequencies, we get:

$$\begin{aligned}\varepsilon_2(\omega_{TO}) &= \varepsilon_2^{(d)}(\omega_{TO}) + \varepsilon_2^{(s)}(\omega_{TO}) \\ &= a(\varepsilon_0 - \varepsilon_\infty)\gamma_c^{-1}\omega_{TO(c)} \int_o^R e^{-br^2}dr + \frac{|\mu(\omega_{TO})|^2}{\omega_{TO}^2} \times g(\omega_{TO})\end{aligned} \quad (2)$$

where (s) denotes structural. On the other hand, $g(\omega)$ is the phonon density of states and $\mu(\omega)$ is the dipole moment matrix element.

Now, for very low frequencies, we have (see, for example, Ref. [1]):

$$|\mu(\omega)|^2 = k\omega^2(\omega \ll \omega_{TO}) \quad (3)$$

where k is a real constant. For $\omega > \omega_{TO}$, by Eq. (2) it follows:

$$\frac{\varepsilon_2^{(s)}(\omega_{TO})}{g(\omega_{TO})} = \frac{|\mu(\omega_{TO})|^2}{\omega_{TO}^2} > \frac{|\mu(\omega)|^2}{\omega^2} \neq k \quad (4)$$

In addition, phonon density of states is given by (see, for example, Ref. [5]):

$$g(\omega) = (3N)^{-1} \sum_{n=1}^{n} \delta(\omega - \omega_n) \tag{5}$$

Since $\delta(\omega - \omega_n) = \delta(\omega_{TO} - \omega_n)$, by formulae (4) and (5), it follows:

$$\varepsilon_2^{(s)}(\omega_{TO}) \gtrsim \frac{|\mu(\omega)|^2}{3N\omega^2} \sum_{n}^{N} \delta(\omega - \omega_n), \quad (\omega > \omega_{TO}) \tag{6}$$

3. CONCLUSIONS

We have obtained some interesting results for the high-frequency region of the far-infrared range corresponding to a-GaAs; in fact, we have concentrated our attention on the condition $\omega > \omega_{TO}$. At this point, we recall that the magnitude of the dipole moment matrix element for $\omega = \omega_{TO}$ is considerable larger than that for other frequencies [2].

On the other hand, quantitative studies on the high region of the far-infrared margin become useful in order to estimate optical properties of possible optoelectronic devices based upon a-GaAs; in this context, comparison with a-Si and a-Ge is desirable.

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