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Infrared absorption in glasses and their crystalline counterparts

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Abstract

It is demonstrated by means of numerical analysis that absorption of light in glasses in the IR region, $30 \text{ cm}^{-1} \lesssim \omega \lesssim 10^3 \text{ cm}^{-1}$, can be understood in terms of light absorption in their crystalline counterparts. This signifies the important role of local structural motifs (units) present both in glasses and crystals. Decomposition of the coupling coefficient into coherent and incoherent contributions gives insight into the origin of the spectral features of IR absorption. The analysis has been undertaken for classical molecular dynamics models of vitreous silica and its crystalline counterpart, α -cristobalite.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

One of the simplest types of interaction of an external electromagnetic field with solids is the absorption of infrared (IR) light. The frequency of IR light lies in the range $30 \text{ cm}^{-1} \lesssim \omega \lesssim 10^3 \text{ cm}^{-1}$ and thus coincides with typical frequencies of atomic vibrations. Therefore it is natural to expect a resonance type of interaction of light with atomic vibrations in this frequency range, i.e. IR absorption. In crystals, the energy and momentum conservation laws govern the absorption of photons and the latter leads to interaction of light with atomic vibrations of a special type, i.e. with molecular-type vibrations of local structural units (optic phonons). In glasses, the momentum conservation is relaxed due to a lack of translational invariance but atomic vibrations in the IR domain are quite similar to those in their crystalline counterparts in the sense that similar local structural units are present in glasses and thus they vibrate in a similar way. Therefore we might expect that the origin of some spectral features of the IR absorption in glasses can be understood and interpreted in terms of the IR absorption in their crystalline counterparts. The main aim of this paper is to demonstrate that this is indeed the case.

The idea of similarity between some of the structural, electronic and atomic properties in glasses and their crystalline counterparts is not new [1–3]. For example, it has been suggested

that the first sharp diffraction peak originates from the first δ -functional peak in the crystalline static structure factor [4]. The spectra of electronic and vibrational excitations are quite similar in glasses and corresponding crystals (see e.g. [5–7]). Another example of translationally invariant systems used for understanding the behaviour of disordered structures includes lattice models successfully employed for studying, for example, the origin of the boson peak [8]. However, the similarity for light absorption in glasses and their crystalline counterparts has not been investigated in great detail [9].

Theoretically, IR absorption in disordered systems including glasses has been studied in two main directions: (i) analytically within simple lattice [10, 11] and phenomenological [12] models and (ii) numerically within simple [13] or more sophisticated [14–19] models of real glasses. Recently, a simple analytical model for universal features in the far-IR range has been suggested [9].

2. Formalism

The formal description of interaction of light with atomic vibrations in ordered and disordered system was developed several decays ago by Maradudin [20, 21]. Interaction of a macroscopic system of charged particles vibrating about their equilibrium positions in a solid is described by the Hamiltonian $\hat{H}_{\text{int}} = -\hat{\mathbf{M}} \cdot \mathbf{E}(t)$, where $\hat{\mathbf{M}}$ is the induced dipole-moment operator of the system and $\mathbf{E}(t) = \mathbf{E}_0 e^{-i\omega t}$ is an external monochromatic (of frequency ω) electric field with amplitude \mathbf{E}_0 . In a solid, the external electromagnetic field interacts both with the charged atomic cores (atoms) and the valence electrons, influencing their motion. The atomic and electronic motions are characterized by significantly different timescales (or frequencies). Atomic frequencies lie in the terahertz range ($E_{\text{vibr}} \lesssim 0.1$ eV) while electronic frequencies are typically two orders of magnitude higher. This difference in the timescales allows the electronic degrees of freedom to be treated adiabatically, so that their instantaneous response to the electromagnetic field leads to screening effects for the electromagnetic field acting on the ions. This model is called the rigid-ion model, in which the screening electronic effects are taken into account by introducing effective time-independent ionic charges, q_i , and by replacing the speed of light, c , by $c/\sqrt{\varepsilon_\infty}$, where ε_∞ is the high-frequency limit of the ionic dielectric constant, so that $\hat{\mathbf{M}} = \sum_i q_i \hat{\mathbf{u}}_i$ with $\hat{\mathbf{u}}_i$ being the displacement operator for an atom i from its equilibrium position and the sum is taken over all the atoms in the system.

Interaction of the electromagnetic field with a solid leads to polarization of the solid characterized by the polarization vector $\langle \hat{\mathbf{p}}(t) \rangle = V^{-1} \langle \hat{\mathbf{M}}(t) \rangle$ (where V stands for the volume of the solid and angular brackets mean thermodynamic averaging), which, according to the linear response theory [22], is proportional to the strength of the field $\langle \hat{p}_\alpha \rangle(t) = \chi_{\alpha,\alpha'} E_{\alpha'}(t)$. The linear absorption coefficient of light, $\alpha(\omega)$, is related to the dielectric susceptibility tensor $\chi_{\alpha,\alpha'}$ as $\alpha(\omega) = (4\pi\omega/(3c\sqrt{\varepsilon_\infty})) \text{Im Tr}(\chi(\omega))$. It is easy to show [20] that, in harmonic approximation for atomic vibrations, the expression for $\alpha(\omega)$ can be written in the following form:

$$\alpha(\omega) = \frac{2\pi^2 n}{c\sqrt{\varepsilon_\infty}} \left| \sum_i \frac{q_i}{\sqrt{m_i}} \mathbf{e}_i(\omega) \right|^2 g(\omega), \quad (1)$$

where $\mathbf{e}_i(\omega)$ is the component of the vibrational eigenvector of frequency ω corresponding to atom i of mass m_i , $g(\omega) = (3N)^{-1} \sum_j \delta(\omega - \omega_j)$ (j runs over all the eigenfrequencies) stands for the vibrational density of states (VDOS) and $n = N/V$ is the atomic concentration. As follows from equation (1), the IR absorption coefficient is proportional to the VDOS, $\alpha(\omega) = C_{\text{IR}}(\omega)g(\omega)$. The coefficient of proportionality, $C_{\text{IR}}(\omega)$, is called the coupling

coefficient,

$$C_{\text{IR}}(\omega) = \frac{2\pi^2 n}{c\sqrt{\varepsilon_\infty}} \left| \sum_i \frac{q_i}{\sqrt{m_i}} \mathbf{e}_i(\omega) \right|^2 \equiv \frac{2\pi^2 n}{c\sqrt{\varepsilon_\infty}} \sum_{i,i'} \frac{q_i q_{i'}}{\sqrt{m_i m_{i'}}} (\mathbf{e}_i(\omega) \cdot \mathbf{e}_{i'}(\omega)), \quad (2)$$

and the study of its frequency dependence is one of the challenging tasks in the area of disordered systems (see e.g. [9]).

Equation (1) has been derived without the use of any symmetry properties of the structure and thus it is valid both for ordered and disordered systems. The difference between glasses and crystals is encoded in the expression for the eigenvectors and atomic charges. In crystals, the eigenvectors are phonons (plane waves) and the charges are δ -functionally distributed. In glasses, the eigenvectors are no longer plane waves (their structure is quite complicated [23–25]) and the charges are randomly distributed [9, 16, 18, 19]. Using translational invariance of the crystals, in the case of a crystal having N_{uc} unit cells each containing n_{uc} atoms, equation (1) for the linear absorption coefficient can be recast in the following form [20],

$$\alpha(\omega) = \frac{6\pi^2}{cV\sqrt{\varepsilon_\infty}} \sum_{\mathbf{k}j} \left| \frac{1}{\sqrt{N_{\text{uc}}}} \sum_{\mathbf{n}} e^{i\mathbf{k}\cdot\mathbf{n}} \sum_i^{n_{\text{uc}}} \frac{q_i}{\sqrt{m_i}} \mathbf{e}_i^j(\mathbf{k}) \right|^2 \delta(\omega - \omega_{\mathbf{k}j}), \quad (3)$$

where phonons are characterized by a wavevector \mathbf{k} and phonon-branch number j . The summation over the cell vectors, \mathbf{n} , in the above expression gives $\sum_{\mathbf{n}} e^{i\mathbf{k}\cdot\mathbf{n}} = \delta_{\mathbf{k}+\mathbf{G},0}$ in the long-wavelength limit for the incident light, with \mathbf{G} being the reciprocal-lattice vector. If a finite value \mathbf{Q} of the IR irradiation wavevector is taken into account, then the term $\delta_{\mathbf{k}+\mathbf{G},0}$ should be replaced by $\delta_{\mathbf{k}+\mathbf{G},\mathbf{Q}}$, which reflects momentum conservation in the IR absorption process occurring in the crystal. This is a particular feature of crystals due to the wave character of the vibrational eigenmodes being characterized by a certain value of momentum, and it is absent in disordered structures. The final expression for the linear absorption coefficient in the crystalline case then reads

$$\alpha(\omega) = \frac{6\pi^2}{cV_{\text{uc}}\sqrt{\varepsilon_\infty}} \sum_j \left| \sum_i^{n_{\text{uc}}} \frac{q_i}{\sqrt{m_i}} \mathbf{e}_i^j(0) \right|^2 \delta(\omega - \omega_{0j}), \quad (4)$$

where V_{uc} is the volume of the unit cell. It follows from equation (4) that IR absorption in crystals occurs only at discrete frequencies corresponding to different vibrational branches in the centre of the Brillouin zone ($\mathbf{k} = 0$). Moreover, the three acoustic branches give zero contribution to the IR absorption because, in the long-wavelength limit, the displacements of all atoms in the acoustic waves are the same, i.e. $\mathbf{e}_i^j/\sqrt{m_i}$ does not depend on i and electro-neutrality within the unit cell gives rise to $\sum_i^{n_{\text{uc}}} q_i \mathbf{e}_i^j(0)/\sqrt{m_i} = 0$ for the acoustic branches. In contrast, for other branches (optic) in the long-wavelength limit, the atoms vibrate in an out-of-phase manner, maintaining the centre of mass for a unit cell at a fixed position and thus these contribute to the IR absorption of light.

The extension of the simple rigid-ion model is the polarizable-ion model [16, 18, 19] in which the polarization effects are taken into account. The key feature of the model is in accurate calculation of the polarization vector $\hat{\mathbf{p}}(t)$ using the more general (tensor) relation connecting the polarization with atomic displacements,

$$\hat{p}_\alpha = \sum_i \frac{\partial \hat{p}_\alpha}{\partial u_{i\alpha'}} u_{i\alpha'} \equiv V \sum_i Z_{i,\alpha\alpha'} u_{i\alpha'}, \quad (5)$$

where $Z_{i,\alpha\alpha'}$ is the Born effective charge tensor for atom i . The effective charge tensors can be calculated from first principles [16, 26]. These effective charge tensors replace the atomic

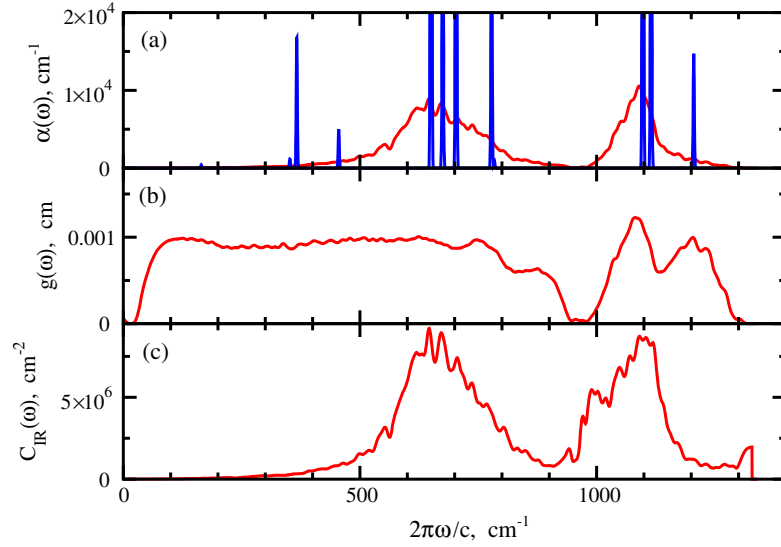


Figure 1. The linear absorption coefficient, $\alpha(\omega)$ (a), vibrational density of states, $g(\omega)$ (b), and coupling coefficient, $C_{\text{IR}}(\omega)$ (c), versus frequency calculated within the rigid-ion approximation for a classical molecular-dynamics model of vitreous silica [24]. The linear absorption coefficient for a classical molecular-dynamics model of α -cristobalite (crystalline counterpart for vitreous silica) is shown in (a) by the vertical lines representing δ -functional peaks.

charges q_i in all the formulae given above in a straightforward manner, e.g. the expression for the absorption coefficient (see equation (1)) becomes

$$\alpha(\omega) = \frac{2\pi^2 n}{c \sqrt{\epsilon_\infty}} \sum_{\alpha} \left| \sum_{i\beta} \frac{Z_{i,\alpha\beta}}{\sqrt{m_i}} e_{i\beta}(\omega) \right|^2 g(\omega). \quad (6)$$

The polarizable-ion model gives theoretical predictions which fit the experimental data through the whole frequency range usually much better than the rigid-ion model (see below). However, in the low-frequency range $\omega \lesssim 30 \text{ cm}^{-1}$ (far-IR), both models give equally good predictions for the frequency dependence of the linear absorption and coupling coefficients [9].

3. Results

Comparison of equations (1) and (4) shows that the IR absorption spectra for crystals and disordered materials are quite different. The spectrum for a crystal is a discrete set of δ -functions while in disordered systems it is a continuous function of frequency. As an illustration in figure 1(a), we show the IR absorption spectrum of vitreous silica and α -cristobalite (a crystalline counterpart of vitreous silica [23]) calculated for classical molecular-dynamics models [24] of these materials within the rigid-ion model, according to equations (1) and (4). It can be seen from figure 1 that, for crystalline α -cristobalite, the absorption spectrum indeed consists of a collection of δ -functions, indicating the positions of the optic branches at the Brillouin-zone centre (the Γ -point). Only optic modes having a transverse component in the polarization vector can be detected in such a manner by the IR absorption. This follows from the momentum-conservation law and the fact that the electric field in the electromagnetic wave is perpendicular to the direction of propagation of light, and thus purely longitudinal vibrational eigenmodes do not interact with the light. For vitreous silica, the absorption spectrum is a

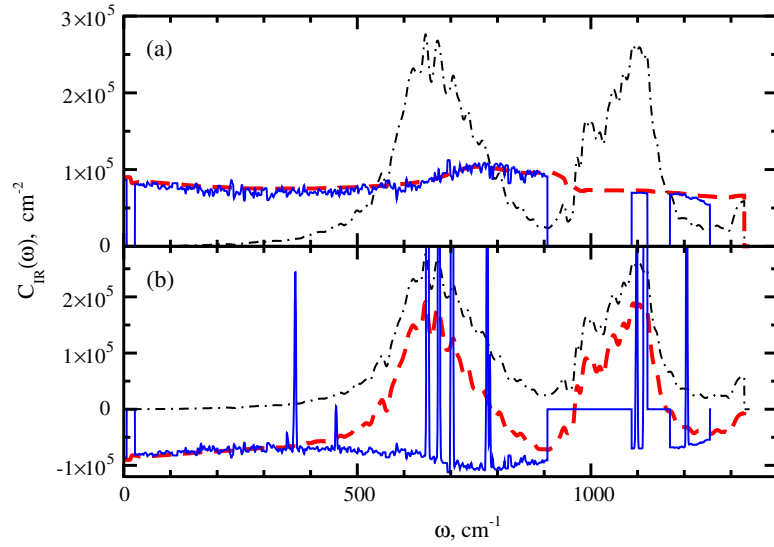


Figure 2. Incoherent (a) and coherent (b) contributions (dashed lines) to the total coupling coefficient (dot-dashed line) for atomic vibrations and infrared photons. The same decomposition of the coupling coefficient for α -cristobalite is shown by the solid lines. The data were obtained for the same models as in figure 1.

continuous function and it can be imagined as being approximately obtained by broadening the δ -functions of the corresponding crystalline counterpart, i.e. of α -cristobalite. The reason for the existence of a continuous IR absorption spectrum in disordered systems is due to the fact that a disordered vibrational eigenmode is not characterized by a unique value of the wavevector [27], as is the case in crystals, and thus IR light having any frequency from the range of vibrational spectrum can be absorbed by an eigenmode of the same frequency (due to energy conservation).

The absorption coefficient is proportional to the vibrational density of states (see equation (1)) but, as seen from figure 1, the shape of the absorption spectrum is quite different from $g_\omega(\omega)$ (cf figures 1(a) and (b)). The reason for this discrepancy is a significant frequency dependence of the coupling coefficient, $C_{\text{IR}}(\omega)$ (see figure 1(c)). The expression for $C_{\text{IR}}(\omega)$ given by equation (2) can be split into two contributions, coherent and incoherent, in exactly the same fashion as for the dynamical structure factor in inelastic-neutron scattering [28], i.e.

$$C_{\text{IR}}(\omega) = C_{\text{IR}}^{\text{incoh}}(\omega) + C_{\text{IR}}^{\text{coh}}(\omega) \\ = \frac{2\pi^2 n}{c\sqrt{\epsilon_\infty}} \sum_i \frac{q_i^2}{m_i} \mathbf{e}_i^2(\omega) + \frac{2\pi^2 n}{c\sqrt{\epsilon_\infty}} \sum_{i \neq i'} \frac{q_i q_{i'}}{\sqrt{m_i m_{i'}}} (\mathbf{e}_i(\omega) \cdot \mathbf{e}_{i'}(\omega)). \quad (7)$$

The incoherent term in equation (7) treats all the atoms as independent absorbing objects in contrast to the coherent one which takes correlation effects into account. The frequency dependence of both contributions for the case of vitreous silica is shown in figure 2. It follows from this figure that both terms contribute, with the main peaks in the spectrum being due to the coherent term for this particular model. This is in marked contrast to the situation for inelastic-neutron scattering where the incoherent part alone makes the dominant contribution [28]. For this model of vitreous silica, the incoherent part of the absorption coefficient is rather featureless and is approximately constant through the whole frequency range of the vibrational spectrum (see figure 2(a)). Moreover, both the disordered material

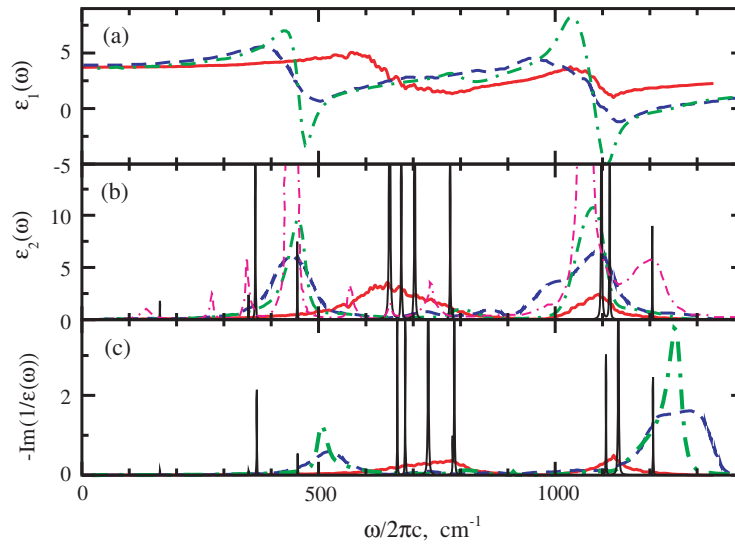


Figure 3. The frequency dependence of the real, $\epsilon_1(\omega)$ (a), and imaginary, $\epsilon_2(\omega)$ (b), parts of the dielectric response function and of $-\text{Im} \epsilon^{-1}(\omega)$ (c) for the classical molecular dynamics model [24] of vitreous silica within the rigid-ion model (the solid curve), for the *ab initio* model of vitreous silica within the polarizable-ion model [18] (the dashed curve) and the experimental data [32] (the dot-dashed curve). The vertical solid lines represent δ -functional response of the classical molecular dynamics model of α -cristobalite and double-dash-dotted line shows the experimental data [33].

and its crystalline counterpart show remarkably similar incoherent absorption profiles (cf the dashed and solid lines in figure 2(a)).

The real difference between the IR absorption in disordered and ordered structures comes from the coherent contribution, at least for this model of vitreous silica. In crystals, this is equal to the negative of the incoherent contribution, so that $C_{\text{IR}}(\omega) = 0$ for practically all frequencies excluding those of the optic modes at the Brillouin zone centre, but in disordered systems such a compensation is not exact in the whole frequency range. Again, it can be seen from figure 2(b) that the positions of the δ -functions for α -cristobalite mainly coincide with the positions of the peaks for silica, thus indicating a tight connection between the two structures. Note that we have found a similar connection in peak positions for *ab initio* based models of As_2S_3 glass and orpiment, its crystalline counterpart [9].

As was mentioned above, the IR absorption in crystals gives information only about the vibrational eigenmodes having the transverse component in the polarization vector. The frequencies of these modes coincide with the poles of the complex dielectric response function, $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega) = (1/3) \text{Tr}(\boldsymbol{\epsilon}(\omega))$, which is related to the dielectric susceptibility tensor, with $\epsilon_{\alpha\beta}(\omega) = \epsilon_{\infty}\delta_{\alpha\beta} + 4\pi\chi_{\alpha\beta}(\omega)$. In disordered systems, both wavevector and polarization vector lose their meanings for atomic vibrations and thus the IR absorption spectrum gives only approximate information about the dominant ‘transverse’ polarization of the eigenmodes. A natural question arises about the possibility of detecting the eigenmodes with (dominant) longitudinal polarization using IR light. The answer to this question is positive and is well established for ionic crystals [29]. Namely, the zeros of the dielectric response function or equivalently the poles of $\epsilon^{-1}(\omega)$ coincide with the eigenfrequencies of the longitudinal vibrational eigenmodes [30]. This means that $\text{Im} \epsilon^{-1}(\omega)$ is of δ -functional shape exactly at the frequencies of the longitudinal vibrational eigenmodes (see figure 3(c)). The positions of

the δ -functional peaks corresponding to the longitudinal phonons are shifted up in frequency with respect to the transverse ones (cf figures 3(b) and (c)). This is a manifestation of the well-known phenomenon of transverse-optic longitudinal-optic phonon frequency splitting in the heteropolar crystalline semiconductors and insulators [29].

The function $\text{Im } \varepsilon^{-1}(\omega)$ is similar to $\text{Im } \varepsilon(\omega)$. Similarly to the IR absorption coefficient, $\alpha(\omega) = \omega \varepsilon_2(\omega) / (c \sqrt{\varepsilon_\infty})$, describing the energy loss of photons due to interactions with transverse phonons, the function $-\omega \text{Im } \varepsilon^{-1}(\omega) / c$, describes the energy loss for an external charge moving fast through the solid (e.g. an electron of energy ~ 10 keV) and creating longitudinal electromagnetic field which interacts with longitudinal electronic excitations, plasmons, in a typical frequency range of ~ 10 eV [31].

In disordered systems, the function $-\text{Im } \varepsilon^{-1}(\omega)$ is continuous in frequency due to the same reasons as for $\text{Im } \varepsilon(\omega)$ (i.e. for the absorption coefficient) but it has a slightly different shape (cf figures 3(b) and (c)). The number of peaks is the same for both functions but their positions for $-\text{Im } \varepsilon^{-1}(\omega)$ are shifted up in frequency thus indicating the splitting between the transverse and longitudinal-optic vibrational modes [13] which is reminiscent to that found in crystals. Of course, the mode classification in disordered systems is not precise because the polarization cannot be strictly defined due to the absence of a definite wavevector for disordered eigenmodes. The positions of the silica peaks both for transverse and longitudinal modes mainly coincide with the positions of the crystalline peaks thus indicating an inherited nature of the glassy spectra.

The numerical evaluation of the dielectric response function, $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, in disordered isotropic media is straightforward once all the eigenmodes are known. More importantly, both real and imaginary parts can be obtained experimentally from optic (e.g. reflectivity and/or transmission) measurements. The experimentally measured real and imaginary parts of the dielectric response functions for vitreous silica are shown in figure 3. The predictions of the rigid-ion model agree at least qualitatively with the experimental data while the polarizable-ion model fits the data rather well. It is worth mentioning that the experimental data for $\varepsilon_2(\omega)$ support the idea of close connection between the glassy and crystalline peak positions (cf the dot-dashed curve for vitreous silica [32] and double-dash-dotted curve for α -cristobalite [33] in figure 3(b)).

Therefore, from optical measurements in the IR region both transverse and longitudinal optical absorption spectra can be obtained (see figures 3(b) and (c)). These spectra can have some bands (peaks). The meaning of these peaks is that the disordered eigenmodes with frequencies from these regions resemble transverse or longitudinal optical phonons closer than the eigenmodes from other regions. This allows us, in some sense, to classify the vibrational eigenmodes in disordered systems.

4. Conclusions

In conclusion, we have presented numerical evidence for a tight connection between IR absorption spectra in silica glass and its crystalline counterpart, α -cristobalite. The frequency dependences of the linear absorption coefficient, the coupling coefficient and dielectric response function in silica have peak-shaped features which can be imagined as originating from the disorder-induced broadening of the corresponding δ -functional peaks in α -cristobalite. The most striking similarity in the responses of silica and α -cristobalite has been found in the incoherent contribution to the coupling coefficient. It has also been demonstrated that analysis of the transverse and longitudinal IR absorption spectra allows the vibrational eigenmodes in disordered systems to be approximately classified in terms of polarization.

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