

Origin of the Boson Peak in Systems with Lattice Disorder

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The origin of the boson peak in models with force-constant disorder has been established by calculations using the coherent potential approximation. The analytical results obtained are supported by precise numerical solutions. The boson peak in the disordered system is associated with the lowest van Hove singularity in the spectrum of the reference crystalline system, pushed down in frequency by disorder-induced level-repelling and hybridization effects.

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The physics of atomic vibrations in crystals is well understood. Disorder produces new features in such dynamics. The van Hove singularities are smeared out, extra states (in addition to the Debye-like acoustic waves) appear in the low-frequency regime (the boson peak) [1], and band tails containing localized vibrations are formed. In this Letter, we discuss the origin of the boson peak, a problem which has attracted a lot of experimental [2,3], simulational [4–8] and analytical [9–12] activity and produced a number of models for it, see, e.g., [8], and references therein, but which is still far from being completely understood.

We chose to study models with lattice disorder [13–15]. In such models, the atoms occupy ideal crystalline positions, but, for example, are connected by springs characterized by spring constants, κ , distributed according to a certain probability distribution, $\rho(\kappa)$. This choice was dictated by two reasons: (i) these models have the simplest type of disorder and should reveal all the salient features, with the existence of positional disorder not expected to make a qualitative difference; (ii) there is a well-developed analytical approach, the coherent potential approximation (CPA), for such models having crystalline reference structures [14–19].

The CPA method is known to work very well for a wide class of problems in the energy range where the eigenstates are not localized. In our case, the vibrational modes in the low-frequency regime (the boson-peak range and below) are found not to be localized [20] (these could be resonant states [8,21]), so that CPA should be valid. Below, we develop the CPA method for vector atomic vibrations in structural models with force-constant disorder (the boson peak in a scalar model with spring constant disorder has been studied in Ref. [6]), obtain the vibrational density of states (VDOS) in the whole frequency range, including the boson-peak region, and demonstrate the reliability of the CPA by comparing it with precise numerical results. This analytical approach allows us to understand and describe quantitatively the origin of the boson peak in terms of disorder-induced level-repelling and hybridization effects which are general in nature and should play a similar role in positionally disordered structures, although the formalism

described below is not straightforwardly applicable for the case of positional disorder.

We treat the problem in the harmonic approximation when the classical description is adequate [14], and the system can be characterized by the Hermitian dynamical operator, $\hat{\mathbf{D}} = \sum_{(i\alpha)(j\beta)} \mathbf{D}_{(i\alpha)(j\beta)} (|i, \alpha\rangle - |j, \alpha\rangle) (\langle i, \beta| - \langle j, \beta|)$, with $|i, \alpha\rangle$ being the site basis describing the displacement of atom i along the Cartesian direction α . The matrix elements, $\mathbf{D}_{(i\alpha)(j\beta)} = (\kappa_{ij}/2) (\hat{\mathbf{r}}_{ij})_{\alpha} (\hat{\mathbf{r}}_{ij})_{\beta}$ (for $i \neq j$), obeying the sum rule, $\sum_j \mathbf{D}_{(i\alpha)(j\beta)} = 0$ [22], are defined in terms of spring constants, κ_{ij} , and unit vectors, $\hat{\mathbf{r}}_{ij}$, connecting the nearest-neighbor atoms i and j (of unit masses). The eigenvalues (“energies”), ε , of the dynamical operator are nonnegative definite, $\varepsilon = \omega^2 \in [0, \infty)$, with ω being the eigenmode frequency.

The basic idea of the CPA is to reduce the problem to that with a known solution, namely, the problem of an effective crystal, where the atoms are connected by identical springs characterized by an unknown (possibly complex) spring constant, $\tilde{\kappa} = \tilde{z} \kappa_0$, with κ_0 being the average spring constant in the real crystal around which the spring constants are distributed in disordered structures ($\kappa_0 = 1$ below). The dimensionless effective spring constant, \tilde{z} , can be found from the self-consistent equation which results from the requirement that the solution for the effective crystal with one spring constant, z , chosen from a random set (single-bond approximation [14,16,17]) averaged over the distribution of z , coincides with the solution for the perfect effective crystal:

$$\left\langle \frac{(z - \tilde{z})}{1 - (z - \tilde{z})\alpha(\varepsilon, \tilde{z})} \right\rangle = 0. \quad (1)$$

Here the configurational averaging ($\langle \dots \rangle$) is over the distribution of the dimensionless disordered spring constants, $z = \kappa/\kappa_0$. For definiteness, we consider below a box distribution for $z \in [1 - \Delta, 1 + \Delta]$. (The choice of other distributions, e.g., normal, does not change the results qualitatively.) The function $\alpha(\varepsilon, \tilde{z})$ is completely defined by the properties of the reference crystalline structure and can be easily derived using the results of Ref. [19],

$$\alpha(\varepsilon, \bar{z}) = \frac{2D}{Z\bar{z}} \left[\frac{\varepsilon}{\bar{z}} G^{\text{cryst}}\left(\frac{\varepsilon}{\bar{z}}\right) - 1 \right], \quad (2)$$

where Z is the number of nearest neighbors, D is the space dimensionality in the case of vector vibrations, and $D = 1$ for scalar vibrations independent of the space dimensionality (see, e.g., [6]). The function $G^{\text{cryst}}(x) = \int_0^\infty g_\varepsilon^{\text{cryst}}(\varepsilon)(x - \varepsilon)^{-1} d\varepsilon$ [with $g_\varepsilon^{\text{cryst}}(\varepsilon)$ being the crystalline VDOS] in Eq. (2) is an analytical continuation of the crystalline Green function to the upper half of the complex plane (see, e.g., [14]).

The quantity of interest is the VDOS for the disordered structure, $g_\varepsilon^{\text{dis}}(\varepsilon)$ which, within the CPA, obeys the following equation:

$$g_\varepsilon^{\text{dis}}(\varepsilon) = -\frac{1}{\pi} \text{Im} \left[\frac{1}{\bar{z}} G^{\text{cryst}}\left(\frac{\varepsilon}{\bar{z}}\right) \right], \quad (3)$$

with $\bar{z}(\varepsilon) = \bar{z}' + i\bar{z}''$ being found self-consistently from Eq. (1). This can be easily done numerically in the whole energy range, but in the low-energy limit ($\varepsilon \rightarrow 0$) analytical results can be derived. For small levels of disorder ($\Delta \ll 1$), the real part of the effective spring constant is close to unity, $\bar{z}' = 1 - (2D/3Z)\Delta^2[1 + O(\varepsilon)]$. For arbitrary disorder, $\bar{z}'(\varepsilon)$ slowly approaches a constant value as $\varepsilon \rightarrow 0$, being the largest root of the equation which follows from Eq. (2) for a box distribution of spring constants, $4D\Delta/Z\bar{z}' = \ln[(1 + \Delta + \gamma\bar{z}')/(1 - \Delta + \gamma\bar{z}')] (with $\gamma = Z/2D - 1$). This equation has a solution, $\bar{z}'(\varepsilon = 0, \Delta)$, only for values of disorder which are not too large, i.e., $\Delta \leq \Delta_*$. The critical disorder, Δ_* , can be found numerically; e.g., for an fcc reference crystal, $\Delta_* \approx 1.296$ and $\bar{z}'_* = \bar{z}'(0, \Delta_*) \approx 0.435$. For $\Delta > \Delta_*$, the system becomes unstable (negative eigenvalues appear) because of a large concentration of negative spring constants, which are introduced in the system for $\Delta > 1$.$

The low-energy imaginary part of the effective spring constant, $\bar{z}''(\varepsilon \rightarrow 0)$, approaches zero (if $\Delta \leq \Delta_*$), as $\bar{z}''(\varepsilon) \approx C\varepsilon^{D/2}$ (being a general consequence of the Debye law for the reference crystal). The constant, $C(<0)$, depends on the parameters of the model [23], and, for $\Delta \ll 1$, $C \approx C_0 = -\pi\chi_D(2D/3Z)\Delta^2$ with χ_D being the coefficient in the Debye law for the low-energy spectrum of the reference crystal, $g_\varepsilon^{\text{cryst}}(\varepsilon) \approx \chi_D\varepsilon^{(D/2)-1}$ [22].

Once $\bar{z}(\varepsilon \rightarrow 0)$ is known, the low-energy limit for the VDOS in the CPA follows straightforwardly from Eq. (3) in which $\text{Re}[G^{\text{cryst}}(\varepsilon)] \approx \text{const}$ and $\text{Im}[G^{\text{cryst}}(\varepsilon)] \approx -\pi g_\varepsilon^{\text{cryst}}(\varepsilon/\bar{z}') \approx -\pi\chi_D(\varepsilon/\bar{z}')^{(D/2)-1}$ as $\varepsilon \rightarrow 0$, so that

$$g_\varepsilon^{\text{dis}}(\varepsilon \rightarrow 0) \approx \frac{1}{\bar{z}'} g_\varepsilon^{\text{cryst}}\left(\frac{\varepsilon}{\bar{z}'}\right) \approx \frac{1}{\bar{z}'} \chi_D \left(\frac{\varepsilon}{\bar{z}'}\right)^{(D/2)-1} \quad (4)$$

[see the inset in Fig. 1(a)]. This means, not surprisingly, that in the low-energy regime the VDOS for disordered systems (with $\Delta < \Delta_*$) also satisfies the Debye law ($g_\omega = 2\omega g_\varepsilon \propto \omega^{D-1}$), but the coefficient before the fac-

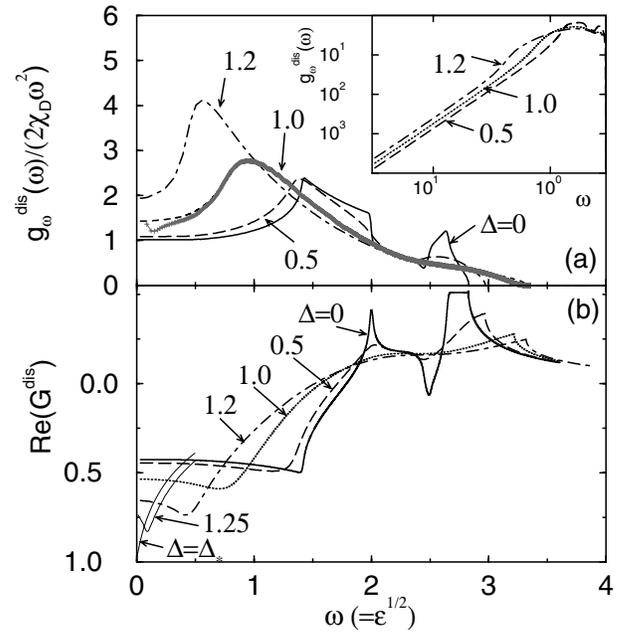


FIG. 1. (a) The reduced VDOS, $g_\omega/(2\chi_D\omega^{D-1})$, for different degrees of force-constant disorder (as marked in the figure) of an fcc structure ($Z = 12$, $D = 3$, vector model). The crosses represent the exact numerical solution by KPM [25] for the fcc reference structure containing $130 \times 130 \times 130$ atoms for vector vibrations with $\Delta = 1$. The inset shows the VDOS, $g_\omega^{\text{dis}}(\omega)$, demonstrating the ω^{D-1} law (here ω^2) in the low-energy part. (b) The real part of the disordered Green function, $\text{Re}[G^{\text{dis}}(\omega^2)]$, versus $\omega = (\varepsilon)^{1/2}$. The critical behavior of $\text{Re}[G^{\text{dis}}(\omega^2)]$ for values of Δ near $\Delta_* = 1.296$ is shown.

tor ω^{D-1} is larger for disordered structures than for the corresponding crystalline reference structure, i.e., $g_\omega^{\text{dis}} \approx (\bar{z}')^{-D/2} g_\omega^{\text{cryst}}$ with $\bar{z}' < 1$ [see the inset in Fig. 1(a)].

In the reference crystal, the reduced VDOS, $[g_\omega/(2\chi_D\omega^{D-1})]$, begins to deviate from unity with increasing frequency and finally exhibits a van Hove singularity [see the peak in the solid curve around $\omega \approx 1.4$ in Fig. 1(a)]. A similar effect occurs in disordered structures. The reduced VDOS shows a greater frequency dependence, eventually resulting in a peak below the van Hove singularity [see Fig. 1(a)], which is called the boson peak [1]. This effect is due to the appearance of extra states in this low-frequency range with a density, $\Delta g_\omega = g_\omega^{\text{dis}} - g_\omega^{\text{cryst}}$, also exhibiting a peak (sometimes called the boson peak as well), the position of which in real glasses is normally close to the position of the peak in the reduced VDOS (see Ref. [24], and references therein). It is clearly seen from Fig. 1(a) that the boson peak is generically related to the lowest van Hove singularity for the reference crystalline structure, which is shifted downwards and broadened by disorder. A trace of this broadened and shifted “singularity” should also be seen in the real part of the Green function, $G^{\text{dis}} = \bar{z}^{-1}G^{\text{cryst}}(\varepsilon/\bar{z})$. Indeed [see Fig. 1(b)], $\text{Re}[G^{\text{dis}}]$ does show a low-energy minimum (a broadened kink singularity), the position of which is correlated with

the position of the boson peak [cf. Figs. 1(a) and 1(b)]. This low-energy minimum moves downwards in energy with increasing disorder and reaches zero at $\Delta = \Delta_*$, showing typical critical behavior [see Fig. 1(b)] around it (to be discussed elsewhere).

In order to confirm this generic relationship between the boson peak and the lowest van Hove singularity in the reference crystal, we analyze the states, $|d\rangle$, in the disordered structure (e.g., in the boson-peak region) in terms of the bare states, $|\mathbf{k}, \beta\rangle$ (with \mathbf{k} being the wave vector and β numbering the branches), for the reference crystal. Different bare states participate with different weights in a disordered state with energy ε , and the spectral density, $A_{\mathbf{k}\beta}(\varepsilon) = (ND)^{-1} \langle \sum_d |\langle \mathbf{k}, \beta | d \rangle|^2 \delta(\varepsilon - \varepsilon_d) \rangle$, describes these weights [13]. The spectral density, as a function of $\varepsilon_{\mathbf{k}\beta}$, exhibits a single peak around the most probable value and a high-frequency tail (see the dotted line in the inset in Fig. 2). The crystalline states mainly contributing to a

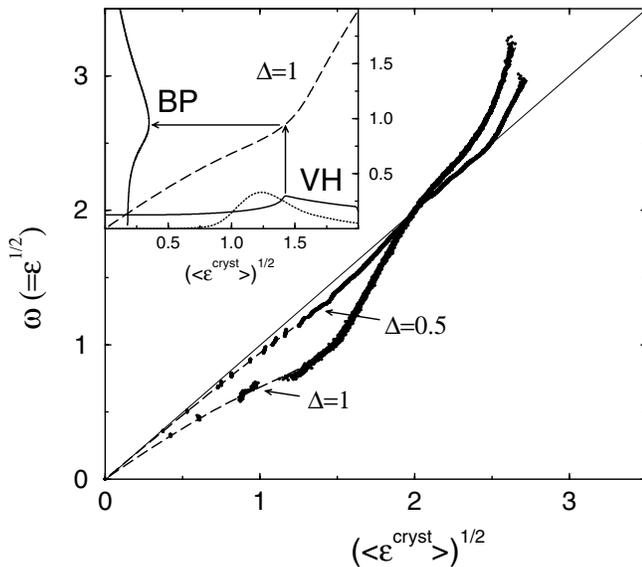


FIG. 2. Disorder-induced level-repelling effect: the frequency of the disordered mode, $\omega = \varepsilon^{1/2}$, versus mean crystalline frequency, $\langle \varepsilon^{\text{cryst}} \rangle = (\langle \varepsilon^{\text{cryst}} \rangle)^{1/2}$ contributing to this disordered mode for different degrees of force-constant disorder, Δ , as marked. Solid circles represent the precise numerical solutions for $12 \times 12 \times 12$ atoms, fcc, vector model; the data in the low-frequency regime are not reliable due to finite-size effects. The level repelling of states, downwards in frequency for $\langle \varepsilon^{\text{cryst}} \rangle \leq 2$ and upwards in frequency at higher frequencies, is evident by reference to the straight line $\omega = \langle \varepsilon^{\text{cryst}} \rangle^{1/2}$. The inset shows the origin of the boson peak: the CPA curve (dashed line) for $\Delta = 1$ is plotted together with the reduced VDOS for the same disordered structure ($\Delta = 1$) along the vertical axis and for the crystal along the horizontal axis (solid curves). The arrows show the connection between the position of the lowest van Hove singularity (VH) and the boson peak (BP) via the CPA results. The dotted curve represents the probability distribution (arbitrarily scaled in height) of weights of the bare states (obtained by direct diagonalization), $g_{\omega}^{\text{cryst}} A_{\mathbf{k}\beta}(\omega^2)$, as a function of the bare state frequency, $\varepsilon_{\mathbf{k}\beta}^{1/2}$ for a disordered state at $\omega = \omega_{\text{BP}} \approx 1$ with the peak position at $(\varepsilon_{\text{max}}^{\text{cryst}})^{1/2}$.

particular disordered state with energy ε can be characterized by the most probable, $\varepsilon_{\text{max}}^{\text{cryst}}(\varepsilon, \Delta)$, and/or average, $\langle \varepsilon^{\text{cryst}}(\varepsilon, \Delta) \rangle = (g_{\varepsilon}^{\text{dis}})^{-1} \sum_{\mathbf{k}\beta} \varepsilon_{\mathbf{k}\beta} A_{\mathbf{k}\beta}(\varepsilon)$, bare energy, which within the CPA has the following form:

$$\langle \varepsilon^{\text{cryst}}(\varepsilon) \rangle \approx \frac{-1}{\pi g_{\varepsilon}^{\text{dis}}(\varepsilon)} \text{Im} \left[\frac{\varepsilon}{\tilde{z}^2} G^{\text{cryst}} \left(\frac{\varepsilon}{\tilde{z}} \right) - \frac{1}{\tilde{z}} \right]. \quad (5)$$

In the region of the mechanical stability of the model ($\Delta < 1$), both of the energies, $\varepsilon_{\text{max}}^{\text{cryst}}$ and $\langle \varepsilon^{\text{cryst}} \rangle$, are close to each other. The results of calculations of $\langle \varepsilon^{\text{cryst}}(\varepsilon) \rangle$ according to Eq. (5) are presented in Fig. 2, from which two conclusions can be drawn. First, the reconstruction of the bare crystalline spectrum by disorder can be described in terms of level-repelling effects (see, e.g., [22]). Indeed, states with $\langle \varepsilon^{\text{cryst}}(\varepsilon) \rangle$ from the low part of the crystalline band are pushed down in energy by predominant level repelling by higher-lying states and hence $\varepsilon < \langle \varepsilon^{\text{cryst}}(\varepsilon) \rangle$ (the dashed lines are below the $\omega = \langle \varepsilon^{\text{cryst}} \rangle$ in Fig. 2 and $\varepsilon < \varepsilon_{\text{max}}^{\text{cryst}}$ in the inset), while the states from the upper part of the band are pushed upwards due to predominant repelling from the bottom states and $\varepsilon > \langle \varepsilon^{\text{cryst}}(\varepsilon) \rangle$. Second, we can check that the states (eigenmodes) in the boson-peak region mainly originate from the bare states located around the lowest van Hove singularity. The inset in Fig. 2 clearly demonstrates this (the difference between $\varepsilon_{\text{max}}^{\text{cryst}}$ and $\langle \varepsilon^{\text{cryst}} \rangle$ is due to the broad high-frequency tail of the spectral density, $A_{\mathbf{k}\beta}$). Therefore, Eq. (5), rewritten in the form, $\langle \varepsilon^{\text{cryst}}(\varepsilon_{\text{BP}}) \rangle \approx \varepsilon_{\text{VH}}$, can serve to estimate the boson-peak position, ε_{BP} , via the position of the lowest van Hove singularity, ε_{VH} . When the disorder approaches the critical value ($\Delta \rightarrow \Delta_*$), the distribution $\Delta g_{\omega}(\varepsilon)$ of extra states in the low-frequency regime (which still mainly originate from the van Hove singularity region) becomes very broad and the position of the peak in $\Delta g_{\omega}(\varepsilon)$ no longer coincides with the position of the peak in the reduced VDOS, resulting in different positions of $\langle \varepsilon^{\text{cryst}}(\varepsilon_{\text{BP}}) \rangle$ (still close to the lowest van Hove singularity) and $\varepsilon_{\text{max}}^{\text{cryst}}(\varepsilon_{\text{BP}})$ (not far above the boson peak); this will be analyzed elsewhere.

Disorder results also in strong hybridization of the bare localized states. This means that a disordered state $|d\rangle$ is comprised of many crystalline bare states $|\mathbf{k}, \beta\rangle$ with energies about $\langle \varepsilon^{\text{cryst}}(\varepsilon) \rangle$ which actually belong to different crystalline branches, β . The relative weights of different branches, w_{β}^{dis} , can be defined within the CPA as $w_{\beta}^{\text{dis}}(\varepsilon) = g_{\varepsilon, \beta}^{\text{dis}}(\varepsilon) / g_{\varepsilon}^{\text{dis}}(\varepsilon)$, via the partial VDOS, $g_{\varepsilon, \beta}^{\text{dis}}(\varepsilon) [g_{\varepsilon}^{\text{dis}}(\varepsilon) = \sum_{\beta} g_{\varepsilon, \beta}^{\text{dis}}(\varepsilon)]$, obeying Eq. (3) in which the crystalline Green function, G^{cryst} , is replaced by the partial one, G_{β}^{cryst} , related to the corresponding partial crystalline VDOS, $g_{\varepsilon, \beta}^{\text{cryst}}$. The results for $w_{\beta}^{\text{dis}}(\varepsilon)$ shown in Fig. 3 demonstrate that the disordered states are indeed comprised of strongly hybridized crystalline states from different branches. The weights for different branches are approximately proportional to the partial crystalline VDOS (actually, smeared out by disorder, cf. the broken lines for the crystal with the solid lines for the disordered structure in Fig. 3). This

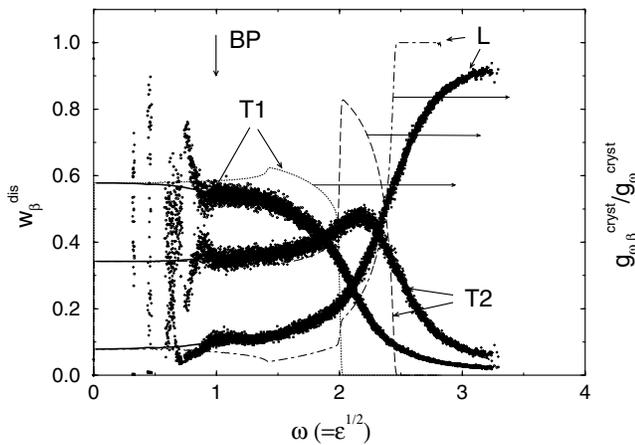


FIG. 3. Branch-hybridization parameters, w_{β}^{dis} ($\beta = 1, 2, 3$ in the case of the fcc model, $12 \times 12 \times 12$), versus frequency, ω , obtained by CPA (solid lines) and by precise numerical analysis (open circles), for a disordered structure with $\Delta = 1$. For comparison, the normalized partial VDOS for each particular branch (two transverse, T1 and T2, and longitudinal, L) in the case of the reference crystal is also shown. The numerical data below $\omega \approx 1$ are unreliable due to finite-size effects.

means that, e.g., for the fcc structure, the disordered states in the region of the boson peak originate mainly from transverse phonons.

We checked the reliability of the CPA approach by calculating the VDOS numerically using the kernel polynomial expansion method (KPM) [25] (see Fig. 1) and level-repelling and hybridization effects by direct diagonalization (see Figs. 2 and 3) and found good agreement across the whole frequency range. We also performed a similar analysis for a 2D triangular lattice and found similar agreement.

In conclusion, we investigated atomic vibrations in disordered systems with force-constant disorder. In such models, (i) the low-frequency VDOS has a Debye-like frequency dependence, albeit with a different coefficient; (ii) the boson peak is related to the lowest van Hove singularity in the spectrum of the reference crystal, shifted downwards in frequency due to level-repelling effects introduced by the disorder; (iii) the disordered vibrational states in the boson-peak region are strongly hybridized crystalline states, with a predominant contribution of that branch which is responsible for the relevant van Hove singularity in the reference crystalline spectrum. This model of the boson peak is based on entirely general effects (level repelling and hybridization), so that we believe it could be extended to topologically disordered structures. At this stage, in a speculative manner, we could assume that the boson peak in topologically disordered structures is related to the lowest van Hove singularities of the corresponding crystalline counterparts (crystals having the same local order as in the disordered systems, e.g., α -cristobalite for silica glass [24], or the σ phase for an icosahedral glass [26]), shifted downwards in frequency by disorder. The types of vibrational modes (acoustic/optic, transverse/lon-

gitudinal) predominant in the boson-peak region are also dictated by the types of phonons responsible for the lowest van Hove singularities in the corresponding crystalline counterpart.

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