Anisotropic interaction of two-level systems with acoustic waves in disordered cubic crystals

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We apply the model introduced by Anghel *et al.* [Phys. Rev. B **75**, 064202 (2007)] to calculate the anisotropy effect in the interaction of two-level systems with phonons in disordered crystals. We particularize our calculations to cubic crystals and discuss the available experimental data. The results presented here provide a way to determine the distribution of the orientations of two-level systems in a disordered crystal, if specific experimental data would be available; for our examples, we assumed isotropic distribution of orientations.

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I. INTRODUCTION

The low-temperature acoustic and thermal properties of amorphous, glassy materials are remarkably similar and they can be explained to a large extent by assuming that the material contains a large number of dynamic defects. These dynamic defects are tunneling systems which are modeled by an ensemble of two-level systems (TLSs).[1,2] Crystals with defects—with a large enough amount of disorder—exhibit also glasslike properties, but these properties are not so universal and, even more, they are not isotropic; for example, the sound absorption and the velocity change depend on the crystallographic direction in which the sound propagates.[3]

Since a detailed microscopic model of tunneling systems in glassy materials is still not available, the study of disordered crystals is especially interesting because it offers an additional opportunity for their clarification: in some materials we know quite well which are the entities that tunnel between different equilibrium positions. Besides this, the anisotropy of the TLS-sound wave interaction in crystals represents another challenge to the interaction models of TLSs which requires clarification.

In this paper we give an explanation for the anisotropy observed in the glasslike properties of general, disordered crystals by employing a model recently published.[4] In this model we assume that each TLS is characterized by a direction in space, call it $\hat{\mathbf{t}}$—this might be the direction defined by the two potential wells of the tunneling system or the axis of rotation of the tunneling entity, and we introduce a coupling between the TLS and a strain field $[S]$, which depends on the amplitude of $[S]$ at the position of the TLS and on the orientation of $\hat{\mathbf{t}}$ with respect to $[S]$. In Ref. 4 the model was applied to an amorphous solid, assuming that the directions $\hat{\mathbf{t}}$ are isotropically distributed, and the effective coupling of an elastic wave with a TLS was calculated as the average over the directions of the TLS. In this way it was proved on very general grounds that, on average, the longitudinal waves couple with the TLSs stronger than the transversal waves—in standard notations $\gamma_l \gtrsim (4/3)\gamma_t$.[4]

In a disordered crystal with TLSs, there could be at least two sources of anisotropy. The first one is that the TLSs might not be anymore isotropically oriented so the effective coupling of elastic waves with them depends, through $\hat{\mathbf{t}}$, on the waves' direction of propagation and on their polarization. The second source of anisotropy is that besides the relative orientation of $\hat{\mathbf{t}}$ and $[S]$, the symmetry of the crystal is manifested also in the interaction of elastic waves with TLSs.[4,5] This leads to anisotropy effects in the interaction of elastic waves with TLS even if the TLS distribution is isotropic.

In this paper we analyze the second source of anisotropy. We shall assume that the TLS orientations are isotropically distributed and we shall calculate the anisotropy effects imposed only by the lattice symmetries onto the interaction Hamiltonian. We shall particularize our calculations to crystals of cubic symmetry, which would enable us to discuss briefly the experimental results of Topp (see Ref. 6 and references therein).

There is not enough experimental data to check the model, but if the results presented in this paper are confirmed or not, we would still constitute a test for the assumption of isotropy of the TLS orientations in a crystal of cubic symmetry.

II. ANISOTROPIC INTERACTION OF TWO-LEVEL SYSTEMS WITH SOUND WAVES

In the standard tunneling model (STM), the Hamiltonian of an isolated TLS is written in a two-dimensional basis as[1,2]

$$H_{\mathrm{TLS}} = \frac{\Delta}{2}\sigma_z - \frac{\Lambda}{2}\sigma_x \equiv \frac{1}{2}\begin{pmatrix} \Delta & -\Lambda \\ -\Lambda & -\Delta \end{pmatrix}, \tag{1}$$

where Δ is called the *asymmetry of the potential* and Λ the *tunnel splitting*. The basis in which the Hamiltonian of Eq. (1) is written is chosen in such a way that a perturbation to the TLS, caused by a strain field, say, $[S]$, is described by a diagonal Hamiltonian

$$H_1 = \frac{1}{2}\begin{pmatrix} \delta & 0 \\ 0 & -\delta \end{pmatrix}, \tag{2}$$

with $\delta \equiv 2[\gamma]:[S]$ and $[\gamma]$ a second-rank tensor of coupling constants; by ":" we denote the dyadic product. Typically, in the STM one considers the coupling of TLSs with transversely or longitudinally polarized sound waves, so not too much attention has been given to the $[\gamma]$ tensor and in general δ is written simply as $\delta=2\gamma_{l,t}S_{l,t}$, with γ and S being scalars (S is the amplitude of the strain field) and l and t denoting the longitudinal (l) or the transversal (t) polarization of the sound wave, respectively. Such a simple description of the TLS-strain field interaction has several shortcomings, e.g., δ is not invariant and even leads to physical ambiguities at the rotation of the coordinates axes, and cannot account for the anisotropy of the TLS-phonon interaction in disordered crystals. As a consequence, in Ref. 4 we proposed a model which eliminates the shortcomings and takes into account the symmetries of the material in which the TLSs are embedded and the orientation of the TLS with respect to the strain field. Let us describe briefly how this is done.

We construct from the components of $\hat{\mathbf{t}}$ the simple 3×3 symmetric tensor $[T]$ of components $T_{ij}=t_it_j$ and we introduce the fourth rank tensor of TLS-strain field coupling constants $[[R]]$. With these two objects, we build the general tensor $[\gamma]$, as $\gamma_{ij}=T_{kl}R_{klij}$—throughout this paper we assume *summation over the repeated indices*. The fourth rank tensor $[[R]]$ has a similar structure as the fourth rank tensor $[[c]]$ of stiffness constants and reflects the symmetries of the crystal that contains the TLS.[4,7]

For the convenience of the calculations we work here, like in Refs. 4, 5, and 7, in abbreviated subscript notations and write $[T]$ and $[S]$ as the six elements vectors $\mathbf{T}\equiv(T_{11},T_{22},T_{33},2T_{23},2T_{13},2T_{12})^t$ and $\mathbf{S}\equiv(S_{11},S_{22},S_{33},2S_{23},2S_{13},2S_{12})^t$, where by "$\cdot^t$" we denote the transpose. Following the notations of Auld,[8] the components of the symmetric tensors will be denoted in abbreviated subscript notations by a single, upper case subscript, e.g., T_I, S_I, and $T_3\equiv T_{33}=t_3^2$; also in abbreviated subscript notations, the tensors $[[R]]$ and $[[c]]$ will be written as 6×6 matrices $[R]$ and $[c]$ of components R_{IJ} and c_{IJ}, respectively. Putting all these together we get the expression $\delta=2\mathbf{T}^t\cdot[R]\cdot\mathbf{S}$.[4,5,7]

Having now the full expression for the interaction Hamiltonian H_1, we can calculate the amplitude of excitation of a TLS, of parameters Δ and Λ, by a phonon of wave vector $\mathbf{k}$ and polarization σ; we denote by $n_{\mathbf{k}\sigma}$ the number of phonons on the mode $(\mathbf{k},\sigma)$ after the TLS excitation process. The displacement field of the phonon $\mathbf{u}_{\mathbf{k}\sigma}$ is normalized to $N_{\mathbf{k}\sigma}\equiv\sqrt{\hbar/(2V\rho\omega_{\mathbf{k}\sigma})}$ and has the strain field $\mathbf{S}_{\mathbf{k}\sigma}=\nabla_S\mathbf{u}_{\mathbf{k}\sigma}$ (where by ∇_S we denote the *symmetric gradient*, whereas ρ and V are the density and the volume of the solid). This way we get

$$\langle n_{\mathbf{k}\sigma},\uparrow|\widetilde{H}_1|n_{\mathbf{k}\sigma}+1,\downarrow\rangle_{\mathbf{u}_{\mathbf{k}\sigma}}=-\frac{\Lambda}{\epsilon}\sqrt{n_{\mathbf{k}\sigma}}\mathbf{T}^t\cdot[R]\cdot\mathbf{S}_{\mathbf{k}\sigma}, \quad (3)$$

where $\epsilon=\sqrt{\Delta^2+\Lambda^2}$ is the *excitation energy of the TLS*. Therefore the phonon-scattering rate by a TLS in the ground state is

$$\Gamma_{\mathbf{k}\sigma}(\hat{\mathbf{t}})=\frac{2\pi}{\hbar}\frac{\Lambda^2 n_{\mathbf{k}\sigma}}{\epsilon^2}|\mathbf{T}^t\cdot[R]\cdot\mathbf{S}_{\mathbf{k}\sigma}|^2\delta(\epsilon-\hbar\omega). \quad (4)$$

The main characteristic of the TLS-elastic strain interaction is contained in the quantity $M_{\mathbf{k},\sigma}(\hat{\mathbf{t}})\equiv\mathbf{T}^t\cdot[R]\cdot\mathbf{S}_{\mathbf{k}\sigma}$, which we shall calculate next.

As mentioned above, $[R]$, like $[c]$, reflects the symmetries of the lattice. The most general type of lattice is triclinic, in which case $[R]$ is a symmetric matrix containing 21 independent elements. Such a lattice is very complex and in general does not sustain simple transversely or longitudinally polarized elastic waves, but instead, the elastic waves propagating through the crystal will be complex superpositions of longitudinally and transversely polarized plane waves. So, to start with a simpler case and also to be able to compare our calculations with available experimental data,[6] we shall focus in this paper on lattices of cubic symmetry. The tensor $[R]$ for the cubic lattice is very similar to the one for an isotropic material,[4,5,7] but it contains three independent constants instead of two, such as in the isotropic case. So we can preserve the notations of Refs. 4, 5, and 7 and write

$$[R]=\tilde{\gamma}\cdot\begin{pmatrix}1&\zeta&\zeta&0&0&0\\ \zeta&1&\zeta&0&0&0\\ \zeta&\zeta&1&0&0&0\\ 0&0&0&\xi&0&0\\ 0&0&0&0&\xi&0\\ 0&0&0&0&0&\xi\end{pmatrix}, \quad (5)$$

without imposing the isotropy constraint $\zeta+2\xi=1$; similarly, the tensor of elastic stiffness constants is

$$[c]=\begin{pmatrix}c_{11}&c_{12}&c_{12}&0&0&0\\ c_{12}&c_{11}&c_{12}&0&0&0\\ c_{12}&c_{12}&c_{11}&0&0&0\\ 0&0&0&c_{44}&0&0\\ 0&0&0&0&c_{44}&0\\ 0&0&0&0&0&c_{44}\end{pmatrix}. \quad (6)$$

Using $[c]$ we can write the Christoffel equation to find $\mathbf{u}$ and $\mathbf{S}$ for the elastic waves propagating in different directions and then we can calculate M for any $\hat{\mathbf{t}}$, Δ, and Λ. In the end, we average over the ensemble of TLSs to determine the attenuation of the elastic wave or the scattering rate of the phonon. We shall apply this procedure for strain fields corresponding to elastic waves propagating along the crystallographic directions $\langle100\rangle$, $\langle110\rangle$, and $\langle111\rangle$ of the cubic lattice. Along these directions, the cubic lattice can sustain simple, longitudinally, and transversely polarized elastic waves for any allowed values of the parameters c_{11}, c_{12}, and c_{44}.

Solving the Christoffel equations we find that the sound velocities of the longitudinal waves propagating in the $\langle100\rangle$, $\langle110\rangle$, and $\langle111\rangle$ directions are $c_{l,\langle100\rangle}=\sqrt{c_{11}/\rho}$, $c_{l,\langle110\rangle}=\sqrt{(c_{11}+c_{12}+c_{44})/\rho}$, and $c_{l,\langle111\rangle}=\sqrt{(c_{11}+2c_{12}+2c_{44})/\rho}$, respectively. Similarly, the sound velocities of the transversal waves propagating in the $\langle100\rangle$ and $\langle111\rangle$ directions are $c_{t,\langle100\rangle}=\sqrt{c_{44}/\rho}$ and $c_{t,\langle111\rangle}=\sqrt{(c_{11}-c_{12}-c_{44})/\rho}$, respectively, whereas for the transversal waves propagating in the $\langle110\rangle$ direction the sound velocity depends on the direction of polarization: if the wave is polarized in the $\langle100\rangle$ direction (and perpendicular to the direction of propagation), the sound velocity is $c_{t,\langle110\rangle}^{\langle100\rangle}=\sqrt{c_{44}/\rho}$, and if the wave is polarized in the

$\langle 110\rangle$ direction (and also perpendicular to the direction of propagation), the sound velocity is $c_{t,\langle 110\rangle}^{\langle 110\rangle}=\sqrt{(c_{11}-c_{12}-c_{44})/\rho}$. Now we can calculate M for these three directions of propagation.

Since the three directions $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are equivalent, let us take the $\langle 100\rangle$ direction as the $\hat{\mathbf{z}}$ direction. We also define $\hat{\mathbf{t}}$ by the angles θ (nutation) and ϕ (precession) as $\hat{\mathbf{t}}\equiv(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)^t$. With these conventions, we get for the longitudinal wave $\mathbf{u}_{k\hat{\mathbf{z}},l}(\mathbf{r})=N\hat{\mathbf{z}}e^{ik\hat{\mathbf{z}}\cdot\mathbf{r}}$,

$$M_{k\hat{\mathbf{z}},l}=ik\tilde{\gamma}N_{k\hat{\mathbf{z}},l}[\zeta+\cos^2\theta(1-\xi)], \tag{7a}$$

(to simplify the expressions without reducing the clarity, we shall always drop the exponential from the expressions of M and the subscripts of N; the implicit subscripts of N are always the same as the ones of M and $\mathbf{u}$) and for the two reciprocally perpendicular transversal waves $\mathbf{u}_{k\hat{\mathbf{z}},t,x}(\mathbf{r})=N\hat{\mathbf{x}}e^{ik\hat{\mathbf{z}}\cdot\mathbf{r}}$ and $\mathbf{u}_{k\hat{\mathbf{z}},t,y}(\mathbf{r})=N\hat{\mathbf{y}}e^{ik\hat{\mathbf{z}}\cdot\mathbf{r}}$,

$$M_{k\hat{\mathbf{z}},t,x}=ik\tilde{\gamma}\xi N\sin(2\theta)\cos(\phi), \tag{7b}$$

$$M_{k\hat{\mathbf{z}},t,y}=ik\tilde{\gamma}\xi N\sin(2\theta)\sin(\phi). \tag{7c}$$

For the waves propagating in the $\langle 111\rangle$ direction we get the following results. For the longitudinal wave $\mathbf{u}_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})/\sqrt{3},l}(\mathbf{r})=N\frac{\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}}}{\sqrt{3}}\exp[ik\frac{\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}}}{\sqrt{3}}\cdot\mathbf{r}]$,

$$M_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})/\sqrt{3},l}=N\frac{ik\tilde{\gamma}}{3}\{[2\sin(2\theta)(\sin\phi+\cos\phi)+2\sin(2\phi)\sin^2(\theta)]\xi+2\zeta+1\}, \tag{8a}$$

and for the two transversal waves

$$\mathbf{u}_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})/\sqrt{3},t,p_1}(\mathbf{r})=N\hat{p}_1\exp\left[ik\frac{\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}}}{\sqrt{3}}\cdot\mathbf{r}\right]$$

and

$$\mathbf{u}_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})/\sqrt{3},t,p_2}(\mathbf{r})=N\hat{p}_2\exp\left[ik\frac{\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}}}{\sqrt{3}}\cdot\mathbf{r}\right]$$

with polarizations $\hat{p}_1=\frac{-\hat{\mathbf{x}}+\hat{\mathbf{z}}}{\sqrt{2}}$ and $\hat{p}_2=\frac{-\hat{\mathbf{x}}+\hat{\mathbf{y}}}{\sqrt{2}}$, we have

$$M_{\frac{k(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})}{\sqrt{3}},t,p_1}=N\frac{ik\tilde{\gamma}}{\sqrt{6}}[2\xi(\cos\theta-\cos\phi\sin\theta)\sin\theta\sin\phi+(\cos^2\theta-\cos^2\phi\sin^2\theta)(1-\zeta)] \tag{8b}$$

and

$$M_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})/\sqrt{3},t,p_2}=N\frac{ik\tilde{\gamma}}{\sqrt{6}}[\sin(2\theta)(\sin\phi-\cos\phi)\xi-\sin^2\theta\cos(2\phi)(1-\zeta)], \tag{8c}$$

respectively.

For the longitudinal wave

$$\mathbf{u}_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}})/\sqrt{2},l}(\mathbf{r})=N\frac{\hat{\mathbf{x}}+\hat{\mathbf{y}}}{\sqrt{2}}e^{ik\frac{\hat{\mathbf{x}}+\hat{\mathbf{y}}}{\sqrt{2}}\cdot\mathbf{r}}$$

propagating in the $\langle 110\rangle$ direction,

$$M_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}})/\sqrt{2},l}=N\frac{ik\tilde{\gamma}}{2}[2\sin(2\phi)\sin^2\theta\xi+(1+\cos^2\theta)\zeta+\sin^2\theta], \tag{9a}$$

and for the two transversal waves propagating in the same direction, $\mathbf{u}_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}})/\sqrt{2},t,p_1'}(\mathbf{r})=N\hat{p}_1'\exp[ik\frac{\hat{\mathbf{x}}+\hat{\mathbf{y}}}{\sqrt{2}}\cdot\mathbf{r}]$ and $\mathbf{u}_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}})/\sqrt{2},t,p_2'}(\mathbf{r})=N\hat{p}_2'\exp[ik\frac{\hat{\mathbf{x}}+\hat{\mathbf{y}}}{\sqrt{2}}\cdot\mathbf{r}]$, with polarizations $\hat{p}_1'=\hat{\mathbf{z}}$ and $\hat{p}_2'=\frac{-\hat{\mathbf{x}}+\hat{\mathbf{y}}}{\sqrt{2}}$, we have

$$M_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}})/\sqrt{2},t,p_1'}=N\frac{ik\tilde{\gamma}\zeta}{\sqrt{2}}\sin(2\theta)(\sin\phi+\cos\phi) \tag{9b}$$

and

$$M_{k(\hat{\mathbf{x}}+\hat{\mathbf{y}})/\sqrt{2},t,p_2'}=N\frac{ik\tilde{\gamma}}{2}\sin^2\theta\cos(2\phi)(\zeta-1), \tag{9c}$$

respectively.

Now we can calculate the phonon's scattering rates by averaging $\Gamma_{\mathbf{k}\sigma}$ of Eq. (4) over the distribution of TLS parameters Δ, Λ, θ, and ϕ, and taking into account the scattering of phonons from and into the mode $(\mathbf{k},\sigma)$. We assume that the parameters Δ and Λ are independent of the parameters θ and ϕ, and their distribution is the standard $P(\Delta,\Lambda)=P_0/\Lambda$, where P_0 is a constant.[1,2] We change the variables Δ and Λ into the variables ϵ and $u\equiv\Lambda/\epsilon$, with the probability distribution $P(\epsilon,u)=P_0/(u\sqrt{1-u^2})$ and we assume that the fraction of excited TLSs, of energy ϵ, is thermal and corresponds to a temperature T: $n_\epsilon^{(\mathrm{TLS})}=(1+e^{\epsilon/k_BT})^{-1}$. The distribution over θ and ϕ, say, $f(\theta,\phi)$, is unknown. Plugging all these quantities into the standard scattering rate calculation, we get

$$\begin{aligned}\tau_{\mathbf{k}\sigma}^{-1}&=\frac{P_0\tanh\left(\frac{\epsilon}{2k_BT}\right)}{2\hbar}n_{\mathbf{k}\sigma}\int_0^\pi\sin\theta d\theta\int_0^{2\pi}d\phi|M_{\mathbf{k}\sigma}\\&\quad\times[\hat{\mathbf{t}}(\theta,\phi)]|^2f(\theta,\phi)\\&\equiv\frac{2\pi P_0\tanh\left(\frac{\epsilon}{2k_BT}\right)}{\hbar}n_{\mathbf{k}\sigma}\langle|M_{\mathbf{k}\sigma}(\hat{\mathbf{t}})|^2\rangle.\otimes\end{aligned} \tag{10}$$

Now, if we would know $f(\theta,\phi)$, we could use the expressions (7), (8), and (9) for M to calculate scattering rates of phonons propagating in the three different directions.

Since we have no microscopic model for $f(\theta,\phi)$, we shall assume that it is constant (i.e., TLSs are isotropically oriented). Then the results obtained for the scattering times can be compared with experimental results to obtain relations between the parameters ζ and ξ. Under this assumption, using Eq. (7a) we calculate the absorption rate of the longitudinally polarized phonons propagating in the $\langle 100\rangle$ direction,

$$\tau_{k\hat{\mathbf{z}},l}^{-1}=\frac{3+4\zeta+8\zeta^2}{15}P_0\tilde{\gamma}^2K\tanh\left(\frac{\epsilon}{2k_BT}\right), \tag{11a}$$

while for the transversely polarized waves, both Eqs. (7b) and (7c) give the same result,

$$\tau^{-1}_{k\hat{\mathbf{z}},t} = \frac{4\xi^2}{15} P_0 \tilde{\gamma}^2 K \tanh\left(\frac{\epsilon}{2k_BT}\right), \tag{11b}$$

where we simplified the notation by introducing the constant $K \equiv 2\pi N^2 n_{\mathbf{k}\sigma} k^2/\hbar$.

Similarly, in the direction $\langle 111 \rangle$ we get

$$\tau^{-1}_{k\frac{(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})}{\sqrt{3}},l} = \frac{5+20\zeta+20\zeta^2+16\xi^2}{45} P_0 \tilde{\gamma}^2 K \tanh\left(\frac{\epsilon}{2k_BT}\right), \tag{12a}$$

and

$$\tau^{-1}_{k\frac{(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})}{\sqrt{3}},t} = \frac{2[(1-\zeta)^2+2\xi^2]}{45} P_0 \tilde{\gamma}^2 K \tanh\left(\frac{\epsilon}{2k_BT}\right), \tag{12b}$$

where again, the two transversely polarized waves Eqs. (8b) and (8c) give the same result.

Finally, for the phonons propagating along the $\langle 110 \rangle$ direction we obtain the average scattering rates

$$\tau^{-1}_{k\frac{(\hat{\mathbf{x}}+\hat{\mathbf{y}})}{\sqrt{2}},l} = \frac{2+6\zeta+7\zeta^2+4\xi^2}{15} P_0 \tilde{\gamma}^2 K \tanh\left(\frac{\epsilon}{2k_BT}\right) \tag{13a}$$

for the longitudinal wave,

$$\tau^{-1}_{k\frac{(\hat{\mathbf{x}}+\hat{\mathbf{y}})}{\sqrt{2}},t,z} = \frac{4\xi^2}{15} P_0 \tilde{\gamma}^2 K \tanh\left(\frac{\epsilon}{2k_BT}\right) \tag{13b}$$

for the transversal wave polarized in the $\hat{p}_1'$ direction, and

$$\tau^{-1}_{k\frac{(\hat{\mathbf{x}}+\hat{\mathbf{y}})}{\sqrt{2}},t,p_2'} = \frac{(\zeta-1)^2}{15} P_0 \tilde{\gamma}^2 K \tanh\left(\frac{\epsilon}{2k_BT}\right) \tag{13c}$$

for the transversal wave polarized in the $\hat{p}_2'$ direction.

Now we write down the STM results for comparison. Writing $\delta_\sigma = 2\gamma_\sigma S_\sigma$, with $\sigma = l$ or t, the expression for the transition rate is[4]

$$(\tau^{(\mathrm{STM})}_{\mathbf{k},\sigma})^{-1} = P_0 \gamma_\sigma^2 K \tanh\left(\frac{\epsilon}{2k_BT}\right). \tag{14}$$

Therefore, if the transition rate (or, more exactly, the sound absorption rate) varies from one direction to another, we say that the product $P_0\gamma_\sigma^2$ depends on the wave's propagation direction. This dependence of the absorption rate on the wave's propagation direction is obvious in the model used here and Eqs. (11a), (11b), (12a), (12b), and (13a)–(13c) give the expressions for the products $P_0\gamma_\sigma^2$'s corresponding to the propagation directions $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$. Notice that if we impose the condition for isotropy $\zeta + 2\xi = 1$, all Eqs. (11a), (11b), (12a), (12b), and (13a)–(13c) reduce to the isotropic expressions of Ref. 4.

Topp (see Ref. 6 and references therein) measured internal friction along the crystallographic directions $\langle 100 \rangle$ and $\langle 111 \rangle$ of the cubic lattice of Ca stabilized zirconium and from the experimental data they concluded that the product $P_0\gamma_t^2$ is the same for the two directions. From this and using Eqs. (11b) and (12b) we obtain the equation $(1-\zeta)^2 = 4\xi^2$, which is satisfied by the isotropy condition $\zeta + 2\xi = 1$. If this is indeed the case (i.e., this is true within the experimental errors), then the products $P_0\gamma_\sigma^2$ are independent on the propagation direction in the material measured in Ref. 6.

Nevertheless, Topp noticed in Ref. 6 another difficulty of the standard interpretations. In the STM, the TLS relaxation time, by absorbing or emitting a phonon, is

$$(\tau^{(\mathrm{TLS})}_{\epsilon,T})^{-1} = \frac{\Lambda^2}{\epsilon^2}\left(\frac{\gamma_l^2}{c_l^5} + \frac{2\gamma_t^2}{c_t^5}\right)\frac{\epsilon^3}{2\pi\rho\hbar^4}\coth\left(\frac{\beta\epsilon}{2}\right) \equiv \frac{\Lambda^2}{\epsilon^2}(\tau^{(\mathrm{TLS})}_{\min,\epsilon,T})^{-1} \tag{15}$$

(see, for example, Refs. 9 and 10), which, for a given TLS energy ϵ and temperature T, attains its maximum $(\tau^{(\mathrm{TLS})}_{\min,\epsilon,T})^{-1}$ when $\Lambda = \epsilon$, and therefore $\Delta = 0$ [we kept explicit the dependence on T in Eq. (15) for reasons that will be clarified shortly]. In this case the strong dependence of $\tau^{(\mathrm{TLS})}_{\min,\epsilon,T}$ on the sound velocities c_t and c_l, which both depend on the phonon's propagation direction, would imply a strong dependence of $\tau^{(\mathrm{TLS})}_{\min,\epsilon,T}$ on the propagation direction. But the relaxational attenuation of an elastic wave of angular frequency ω has two asymptotic regimes, namely, $\omega\tau^{(\mathrm{TLS})}_{\min,\epsilon=2k_BT_{\mathrm{co}},T_{\mathrm{co}}} \ll 1$ for low T and $\omega\tau^{(\mathrm{TLS})}_{\min,\epsilon=2k_BT_{\mathrm{co}},T_{\mathrm{co}}} \gg 1$ for high T, where the attenuation has very different temperature dependences. The two asymptotic regimes are separated by a crossover temperature T_{co} defined by the equation $\omega\tau^{(\mathrm{TLS})}_{\min,\epsilon=2k_BT_{\mathrm{co}},T_{\mathrm{co}}} = \tanh(1)$, which gives

$$T_{\mathrm{co}} = \left[\frac{2\pi\rho\hbar^4\omega}{8k_B^3(\gamma_l^2/c_l^5 + 3\gamma_t^2/c_t^5)}\right]^{1/3}. \tag{16}$$

From the internal friction experiments of Topp T_{co} appears to be independent of the phonon's propagation direction, but according to Eq. (16), this cannot happen unless γ_l and γ_t depend strongly on the propagation direction (see Secs. 3.5.2 and 3.6 in Ref. 6). Since, on the other hand, the product $P_0\gamma_t^2$ is independent of the propagation direction, this would imply that also P_0 depends on the propagation direction, which is very odd—P_0 is proportional to the density of tunneling states and, therefore, is a scalar in the problem.

From our perspective, this puzzle has a simple solution. To put it short, from the scattering rate Eq. (4) one can calculate the TLS relaxation rate, but when summing over the phonon modes we average the anisotropy in the phonon propagation properties.

More clearly, by standard calculations we get from Eq. (4), instead of Eq. (15), the following expression for $\tau^{(\mathrm{TLS})}_{\epsilon,T}$:

$$\begin{aligned}(\tau^{(\mathrm{TLS})}_{\hat{\mathbf{t}},\epsilon,\Lambda})^{-1} &= \frac{\epsilon^3}{2\pi\rho\hbar^4}\frac{\Lambda^2}{\epsilon^2}\coth\left(\frac{\beta\epsilon}{2}\right)\frac{1}{4\pi}\int_0^\pi d\theta_k \\ &\quad\times \sin\theta_k \int_0^{2\pi} d\phi_k \sum_\sigma \frac{|\mathbf{T}^t\cdot[R]\cdot\mathbf{s}|^2}{c^5_{\hat{\mathbf{k}},\sigma}} \\ &\equiv \frac{\Lambda^2}{\epsilon^2}(\tau^{(\mathrm{TLS})}_{\min,\epsilon,\hat{\mathbf{t}}})^{-1}\end{aligned} \tag{17}$$

[where we introduced in the notation the unit vector $\hat{\mathbf{t}}$ to distinguish the relaxation time calculated by Eq. (17) from the STM one, Eq. (15)]. To make the comparison between Eqs. (15) and (17) more clear, we denoted $\mathbf{s} \equiv \mathbf{S}/N$, where N is the phonon's normalization constant. In Eq. (17), the influence of the phonon's propagation anisotropy on $\tau^{(\mathrm{TLS})}$ is eliminated by the average over the directions $\hat{\mathbf{k}}$, defined by the angles θ_k and ϕ_k. Therefore the strong dependence of $\tau^{(\mathrm{TLS})}$ on the sound velocity variation in different propagation directions disappears under the averaging procedure. The only dependence on direction is through $\hat{\mathbf{t}}$, but this is eventually irrelevant since in determining the regime of relaxational attenuation one compares the frequency of the elastic wave with the relaxation rate of the ensemble of TLS and, therefore, with the average of the relaxation rates over the directions $\hat{\mathbf{t}}$.

III. CONCLUSIONS

We applied the formalism introduced in Ref. 4 to describe the interaction of phonon modes (or elastic waves) with the ensemble of two-level systems in a disordered cubic crystal. We showed that the interaction is in general anisotropic and—in the language of the standard tunneling model—the coupling constants γ_l and γ_t may depend on the phonon propagation direction. We focused our calculations on phonons propagating along the crystallographic directions $\langle 100\rangle$, $\langle 110\rangle$, and $\langle 111\rangle$, for which we gave explicit expressions for the phonons' relaxation times.

Using the experimental results of Topp [see Ref. 6 and references therein], namely, that the product $P_0\gamma_t^2$ has the same value for phonons propagating in both crystallographic directions $\langle 100\rangle$ and $\langle 111\rangle$ in cubic Ca stabilized zirconium, we deduced that for this material the matrix of TLS-phonon coupling constants $[R]$ can satisfy the isotropy condition $\zeta + 2\xi = 1$ [see Eq. (5)]. This would imply that $P_0\gamma_t^2$ and $P_0\gamma_l^2$ have the same values in any direction—in which pure transversal or longitudinal waves can be sustained. This condition can be checked experimentally by measuring the attenuation rate of elastic waves propagating along other crystallographic directions or having longitudinal polarization. Such experiments could also help us determine if the distribution of TLS orientations in the crystal is isotropic or not.

We discussed from our model's perspective the relaxation time of a TLS to the phonons' bath and showed that it is not influenced by the anisotropy of the sound propagation in the crystal, which is eliminated by averaging.

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