# The Mössbauer effect in disordered systems containing two-level tunneling systems

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We calculate the Mössbauer effect for nuclei in samples containing two-level tunneling systems and compare the phonon contribution to the Mössbauer effect with the contribution of two-level tunneling systems. We find that at low temperatures the latter is dominates, which leads to a special temperature dependence for the probability of the Mössbauer effect. © *1994 American Institute of Physics.*

As is well known, the Mössbauer effect is the ability of a nucleus bound in a solid to emit or absorb gamma-photons in gamma-transitions without loss of energy through nuclear recoil. The emission and absorption spectra exhibit unshifted lines with an energy exactly equal to that of the gamma-transition, and the width of these lines is equal to, or close to, the natural linewidth. In this case the emission and absorption lines overlap, which makes it possible to observe resonant absorption of gamma-photons.[1]

It has been established that the probability of the Mössbauer effect can be expressed in terms of the normalized density of phonon states. At low temperatures, primarily low-frequency acoustic phonons are excited. Since the density of states of these phonons is low, the probability of the Mössbauer effect grows as the temperature lowers.

The dynamic and kinetic properties of disordered systems at low temperatures ($T \lesssim 1$K) are determined by two-level tunneling systems (TLTS),[2] whose density of states is energy independent. As noted by Phillips,[3] violation of order in a small volume is sufficient for the occurrence of TLTS. Hence the nucleus that emits or absorbs gamma-photons can usually be expected to be in TLTS.

Since the density of states of TLTS is energy-independent and since at low temperatures primarily low-frequency acoustic phonons and low-energy two-level systems are excited, the Mössbauer effect for a nucleus in TLTS may be determined by the two-level systems.

The aim of the present work is to study the Mössbauer effect for a nucleus in TLTS.

A TLTS constitutes an atom or group of atoms that can be in two almost equivalent equilibrium positions. Transition from one position to the other is achieved through tunneling. The main characteristics of a TLTS are the asymmetry energy $\Delta$, the separation $a$ of the two equilibrium position, the height $V$ of the potential barrier, and the tunneling energy $\Delta_0=\hbar\omega_D e^{-\lambda}$, where $\lambda=\sqrt{2mV}\,a/\hbar$, $m$ is the mass of the atom, and $\omega_D$ is the Debye frequency.

The TLTS Hamiltonian is

$$H=\frac{1}{2}\begin{pmatrix} \Delta & -\Delta_0 \\ -\Delta_0 & -\Delta \end{pmatrix}=\Delta s^z-\Delta_0 s^x,$$

where $s^z$ and $s^x$ are Pauli matrices.

Transformation to the representation in which the TLTS Hamiltonian is diagonal is achieved by introducing the unitary operator $U=\exp\{i\varphi s^y\}$, where $\tan\varphi=\Delta_0/\Delta$, and $s^y$ is the $y$-projection of the pseudospin. In this representation the TLTS Hamiltonian assumes the form

$$H=\varepsilon s^z,$$

where $\varepsilon=\sqrt{\Delta^2+\Delta_0^2}$ is the TLTS energy. The probability of the Mössbauer effect is given by the following formula:[1]

$$f=\exp\{-k^2\langle x^2\rangle\},\tag{1}$$

where $k$ is the wave vector of the gamma-photon, and $\langle x^2\rangle$ the mean-square deviation from an equilibrium position. Bearing in mind that a TLTS can be in two almost equivalent equilibrium positions, we can write $x=x_0+as^z$, where $x_0$ is the deviation from an equilibrium position.

In the diagonal TLTS representation for $x$ we can write

$$x=x_0+a\left(s^z\,\frac{\sqrt{\varepsilon^2-\Delta_0^2}}{\varepsilon}+s^x\,\frac{\Delta_0}{\varepsilon}\right).\tag{2}$$

Substituting (2) into (1) and replacing $s^z$ with the respective fluctuation, for a TLTS we obtain

$$f=\exp\left\{-k^2\langle x_0^2\rangle-\frac{k^2a^2}{4}\left(1-p\int_{\varepsilon_0}^{\varepsilon_m}\int_{\Delta_{0\min}}^{\varepsilon}\frac{\sqrt{\varepsilon^2-\Delta_0^2}}{\varepsilon\Delta_0}\tanh^2\frac{\varepsilon}{2k_BT}\,d\varepsilon\,d\Delta_0\right)\right\},$$

where $p$ is the energy-density of states of TLTS, where $p\approx 1/\varepsilon_{\max}\ln(2\varepsilon_{\max}/e\Delta_{0m})$, $\Delta_{0m}$ is the minimum tunneling energy, and $\varepsilon$ and $\varepsilon_{\max}$ are the minimum and maximum TLTS energies, respectively.

Calculations in the approximation in which $k_BT$, $\Delta_{0m}$, and $\varepsilon_0$ are much smaller than $\varepsilon_{\max}$ yield

$$f\approx\exp\left\{-k^2\langle x_0^2\rangle-\frac{k^2a^2}{4}\left[\frac{1}{\ln(2\varepsilon_{\max}/e\Delta_{0m})}+\frac{2k_BT}{\varepsilon_{\max}}\left(1-\tanh\frac{\varepsilon_0}{2k_BT}\right)\right]\right\}.\tag{3}$$

The first term inside the braces gives the phonon contribution to the total probability of the recoilless process, and for $T\ll\theta$ in the Debye model we have[4]

$$k^2\langle x_0^2\rangle=\frac{3R}{2k_B\theta}\left[1+\frac{2\pi^2}{3}\left(\frac{T}{\theta}\right)^2\right],$$

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where $R$ is the recoil energy, $\theta$ is the Debye temperature, and $k_B$ is the Boltzmann constant.

The second term inside the braces in (3) gives the TLTS contribution to the total probability of the recoilless process, with a temperature dependence weaker than that provided by the $k^2\langle x_0^2\rangle$ term. This suggests that at low temperatures the temperature part of the second term inside the braces in (3) is dominates. Hence the temperature dependence of the probability of the recoilless process at low temperatures is determined by TLTS. Let us compare the phonon and TLTS contributions to the total probability of the recoilless process for $Ir^{193}$, $Au^{197}$, and $Eu^{153}$ nuclei present as impurities in solids with a Debye temperature $\theta \sim 1000$ K. The values of the energy of the gamma-photons and the recoil energy are taken from Ref. 4 and are, respectively, 73 keV and $1.5\times 10^{-5}$ keV, 77.3 keV and $1.6\times 10^{-5}$ keV, and 97.4 keV and $3.3\times 10^{-5}$ keV.

In view of this, we have for the phonon contribution

$$f_{\text{ph}}(\text{Ir}^{193}) \approx \exp\{-0.26-0.17\times 10^{-5}T^2\},$$

$$f_{\text{ph}}(\text{Au}^{197}) \approx \exp\{-0.28-0.18\times 10^{-5}T^2\},$$

$$f_{\text{ph}}(\text{Eu}^{153}) \approx \exp\{-0.57-0.38\times 10^{-5}T^2\}.$$

To estimate the TLTS contribution to the total probability of the recoilless process, for the values of the parameters $\varepsilon_{\max}$, $\Delta_{0m}$, and $a$ we take those for dielectric glasses:[5] $\varepsilon_{\max} \sim 10^3$K, $\Delta_{0m} \sim 10^{-2}$K, and $a \sim 10^{-11}$m.

For the TLTS contribution in the temperature interval $\varepsilon_0 < T < \varepsilon_{\max}$ we have

$$f_{\text{TLTS}}(\text{Ir}^{193}) \approx \exp\{-0.35-0.7\times 10^{-2}T\},$$

$$f_{\text{TLTS}}(\text{Au}^{197}) \approx \exp\{-0.4-0.8\times 10^{-2}T\},$$

$$f_{\text{TLTS}}(\text{Eu}^{153}) \approx \exp\{-0.63-0.13\times 10^{-1}T\}.$$

Since the total probability is the product of $f_{\text{ph}}$ and $f_{\text{TLTS}}$, one can easily see that the dominant exponential function is the one with the greater exponent. From this we conclude that the temperature dependence of the recoilless process in disordered systems containing TLTS in the temperature interval $\varepsilon_0 < T \lesssim 10^{\text{K}}$ is determined by the two-level systems.


[1] H. Lipkin, *Quantum Mechanics: New Approaches to Selected Topics*, North-Holland, Amsterdam (1973).

[2] J. L. Black, in *Glassy Metals. I. Ionic Structure, Electronic Transport and Crystallization*, edited by H.-J. Güntherodt and H. Beck, Springer, Berlin (1981).

[3] W. A. Phillips, J. Non-Cryst. Solids **31**, 267 (1978).

[4] V. S. Shpinel', *Resonance of X Rays in Crystals*, Nauka, Moscow (1991) p. 45 [in Russian].

[5] X. Szeftel and H. Alloul, J. Non-Cryst. Solids **29**, 253 (1978).



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