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Correlation between Einstein and Debye Models of Lattice Vibrations for Mössbauer Fraction

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Recently a new method for quantitative Mössbauer analysis was given by Collins /1/, and extended by Bahgat /2/ to include the absorber thickness. In this method the Einstein model of lattice vibrations was applied to calculate the mean square displacement (MSD), the recoilless fraction, and the concentration of the Mössbauer nuclei in the absorbers. In the study of Collins and Cosgrove /3/, and earlier by Mott and Jones /4/, the Debye temperature Θ_D was correlated to the Einstein temperature Θ_E by the relation $\Theta_D = (4/3)\,\Theta_E$.

In the present report we are going to show that this relation does not apply to the recoilless fraction. However, it needs a modification, also we are going to find out a correlation between the MSD of both models, and finally it will be seen that in the method of quantitative Mössbauer analysis applying the Einstein model is far from being a crude estimation.

Following Collin's procedure the MSD in the Einstein solid can be given as

$$\langle x^2\rangle_E = (\hbar^2/4\,Mk)\;T^*/T_o^2\ , \tag{1}$$

where $T^* = T_o \coth(T_o/T)$, kT_o is the zero point energy in the Einstein solid, M is the mass of the Mössbauer nucleus, $\hbar$ is the Planck constant divided by 2π, k is the Boltzmann constant, T is the ambient temperature, and $T_o = (1/2)\,\Theta_E$ by definition.

This can be given in the expanded form

$$\langle x^2\rangle_E = (\hbar^2/4\,Mk\;T_o)\,(T/T_o + T_o/3T - \tfrac{1}{45}(T_o/T)^3 + \ldots)\ ,$$

where for $T \gg T_o$, it can be approximated to

$$\langle x^2\rangle_E = (\hbar^2/4\,Mk)\,(T/T_o^2)\ ,$$

$$= (\hbar^2/Mk)\,(T/\Theta_E^2)\ . \tag{2}$$

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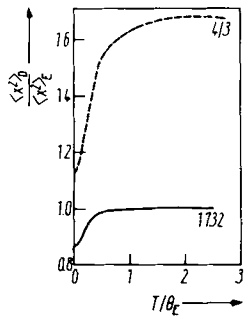

Fig. 1. The relation between $\langle x^2\rangle_D/\langle x^2\rangle_E$ and T/Θ_E for Θ_D/Θ_E = 4/3 (---) and 1.732 (—)

On the other hand, the MSD in the Debye solid can be given as /5/

$$\langle x^2\rangle_D = (3\hbar^2/Mk\,\Theta_D)\left[\frac{1}{4} + (T/\Theta_D)^2 \int_0^{\Theta_D/T} \frac{y\,dy}{e^y - 1}\right] , \tag{3}$$

where at $T \gg \Theta_D$ it is reduced to

$$\langle x^2\rangle_D = (3\hbar^2/Mk)(T/\Theta_D^2) . \tag{4}$$

The recoilless fraction is in general

$$f = \exp(-\langle x^2\rangle/\lambda^2) ,$$

where λ is the gamma-ray wavelength divided by 2π. From (2) and (4) it can be seen that, when $\langle x^2\rangle_E = \langle x^2\rangle_D$:

$$\Theta_D = \sqrt{3}\,\Theta_E . \tag{5}$$

Taking this value to formulate a general relation between both MSD in the whole temperature range, calculations were performed using a TI59 programmable calculator, and applying the continuous Simpson approximation. Fig. 1 shows the results of the calculations for $\langle x^2\rangle_D/\langle x^2\rangle_E$ against T/Θ_E. From this curve (with $\Theta_D/\Theta_E = \sqrt{3}$) the following general relation was deduced to correlate the MSD of both models, and which is applied in the whole temperature range:

$$\langle x^2\rangle_D = \left[1 - \frac{C}{(5T/\Theta_E)^2 + 1}\right] \langle x^2\rangle_E , \tag{6}$$

where C is a constant and equals 0.134.

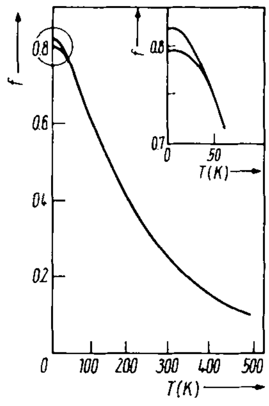

Fig. 2. The calculated recoilless fractions f for both the Einstein and Debye models of lattice vibrations, with $\Theta_E = 100$ K and $\Theta_D = 173.2$ K in case of ^{57}Fe

Fig. 2 shows a representative result of calculating the recoilless fractions for $\Theta_E = 100$ K and $\Theta_D = 173.2$ K. From this figure it can be seen that in the whole temperature range down to 50 K both recoilless fractions are the same. However, below 50 K the deviation is about 2% so that the difference is small and could be recovered on applying (6). On the other hand, it should need a great precision of Mössbauer data.

Consequently, on applying the method of quantitative Mössbauer analysis, the Einstein model for lattice vibrations is quite sufficient for precise results, at least if there is no vibrational anharmonicity or phase transformation in the studied temperature range. However, if there is a contribution from the former only some modifications are needed /6/.

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