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Abstract. A multiphonon mechanism of neutron scattering in glasses is considered. It is due to the interaction of the neutrons with strongly fluctuating double-well potentials characteristic of glasses which may be of importance at not too low temperatures (above the liquid helium temperature). The cross section of this process is calculated and its dependence on the temperature and the neutron energy transfer is found. It is shown that, contrary to the relaxation mechanism, the multiphonon mechanism produces a cross section without a maximum in its temperature dependence. This, as well as some other features, corresponds better to the experimental observations.

1. Introduction

Neutron scattering is an important experimental technique to study vibrational spectra in various solid substances. It allows one, for example, to obtain detailed information concerning the harmonic phonons and local modes in crystals (see, e.g., Maradudin 1966). Recently, attention has also been drawn to the possibility of studying the vibrational spectra of glasses by neutron scattering (Buchenau 1985, Sinclair 1985, Price 1986). Buchenau *et al* (1984) investigated inelastic neutron scattering from vitreous silica in the low energy transfer range, up to a few meV. They have found that, apart from the harmonic phonon contribution, there is excess scattering which is characterized by a structure factor which is independent of the neutron transfer energy. The temperature dependence of the cross section cannot be accounted for by the standard Bose factor (Buchenau *et al* 1988) which means that this excess scattering can hardly be attributed to the harmonic part of the vibrational spectrum. They have also found that the cross section decreases with an increase in the transfer energy.

It is well known now that the spectrum of the glass also contains, apart from the usual harmonic, an anharmonic part. The latter may be represented either by double-well potentials (DWP) or other local anharmonic modes (see, e.g., Phillips 1987, Goldanskii *et al* 1989, Galperin *et al* 1989). We are going to distinguish here, among the various anharmonic modes, the so called rigid DWPs considered in the paper of Fleurov and Trakhtenberg (1986 and references therein) and to calculate their contribution to neutron scattering in the glass.

An important feature of rigid DWPs is that the interaction with them at not too low temperatures (above the liquid helium temperature) has a multiphonon character.

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It is due to the strong fluctuations in the barrier in the DWP which modulate the tunnelling amplitude. We are going to demonstrate here that this mechanism plays an important part in this excess neutron scattering and is capable of explaining its principal features. There are two other mechanisms for scattering in glasses—resonance and relaxation—that have been considered by Maleyev (1986) at low temperatures. At higher temperatures, which are of interest to us here, only the relaxation mechanism may be of importance (Buchenau *et al* 1984, 1988) and can compete with the multiphonon mechanism. The most essential difference in the experimental observation of the two mechanisms is the temperature dependences of the corresponding cross sections. The relaxation cross section is characterized by a maximum which is absent in the multiphonon cross section. This property would help the experimentalist to judge which mechanism is predominant in a particular experiment.

2. Rigid double-well potentials

A brief description of the model for rigid DWPs is given in this section. The aim is to remind us of the principal ideas and to introduce the notation which will be used in the present as well as in the following paper (Fleurov and Levanda 1992). A more detailed account of the model and the calculations can be found in Fleurov and Trakhtenberg (1986), Goldanskii *et al* (1989) and Fleurov (1989).

It is assumed that the principal contribution to various kinetic processes in glasses in the intermediate region of the temperatures is due to the rigid DWPs which contrary to soft DWPs (reviewed by Galperin *et al* 1989) are characterized by the barrier height and width of the atomic order. (Say, the example considered in Fleurov and Trakhtenberg (1986) deals with the barrier height, 0.5 eV, and width, 0.5 Å.) The soft DWPs are responsible for various effects (specific heat, ultrasonic attenuation etc) observed in glasses at low temperatures. However, at higher temperatures (above, say, 10 K) they become ineffective and we have to consider the role of rigid DWPs.

The principal mechanism of the interaction of the phonons with a rigid DWP is due to strong fluctuations (first considered by Kagan and Klinger (1976)) in the barrier shape. The Hamiltonian of the glass is

$$\hat{H} = \sum_i \hat{T}_i + V(\{\boldsymbol{R}_i\}) \tag{2.1}$$

Here $\hat{T}_i$ is the kinetic energy of the ith atom in the glass; $V(\{\boldsymbol{R}_i\})$ is the potential energy of the ensemble of the atoms with the coordinates $\{\boldsymbol{R}_i\}$. Now we have to consider the structure of the wavefunctions of the atomic motion in the glass. The analysis based on the catastrophe theory approach (Karpov *et al* 1982, Fleurov 1990, see also the review of Galperin *et al* 1989) allows one to make a diffeomorphic transformation

$$\{R_i^{\alpha}\} \mapsto \{x_l\}, \{\rho_j\} \tag{2.2}$$

that separates (at least partially) the coordinates, $\{\rho_j\}$, describing the harmonic (phonons) degrees of freedom and the coordinates, $\{x_l\}$, for the anharmonic motions. Some of these anharmonic degrees of freedom correspond to the DWPs and, in particular, to the rigid DWPs which are of a special interest for us in what follows.

In order to proceed further one has to make a double adiabatic approximation whose applicability to rigid DWPs has been discussed in detail in Fleurov and Trakhtenberg (1986) and Goldanskii *et al* (1989). The first stage of this approximation is the

standard Born–Oppenheimer procedure allowing one to separate the electronic $\{r_e\}$ and atomic degrees $\{x_l\}, \{\rho_j\}$ of freedom. The second stage uses the transformation (2.2) and separates the anharmonic $\{x_l\}$ and harmonic $\{\rho_j\}$ degrees of freedom. The interaction with the electronic degrees of freedom takes no part in the neutron scattering, therefore the electron coordinates can be integrated out (they are not even shown in the Hamiltonian (2.1)). Now the wavefunction of the system is represented in the form

$$\Phi_{\alpha,n}(\{x_l\},\{\rho_j\}) = \psi_\alpha(\{x_l\};\{\rho_j\})\Psi_{n;\alpha}(\{\rho_j\}) \tag{2.3}$$

where the wavefunction $\psi_\alpha(\{x_l\};\{\rho_j\})$ describes particles moving in the DWPs at fixed phonon coordinates $\{\rho_j\}$. $\Psi_{n;\alpha}(\{\rho_j\})$ is the phonon wavefunction.

We are going to consider here only independent DWPs which are separated spatially and do not interact directly with each other. Therefore the DWP wavefunction is factorized as

$$\psi_\alpha(\{x_l\};\{\rho_j\}) = \prod_l \psi_{\alpha_l}(x_l;\{\rho_j\})$$

where $\psi_{\alpha_l}(x_l;\{\rho_j\})$ is the wavefunction of the lth DWP and we shall neglect any overlap of the wavefunctions $\psi_{\alpha_l}(x_l;\{\rho_j\})$ for different DWPs. As a result the transition amplitude

$$\langle\psi_{\{\alpha_l\}}(\{x_l\};\{\rho_j\})|V(\{R_i\})|\psi_{\{\beta_l\}}(\{x_l\};\{\rho_j\})\rangle_{\{x_l\}} = \sum_l \Delta_{l,\alpha_l\beta_l}(\{\rho_j\}) \prod_{l'\neq l} \delta_{\alpha_{l'}\beta_{l'}} \tag{2.4}$$

is now the sum of the transition amplitudes for the individual DWPs. Subscript $\{x_l\}$ denotes the integration over the DWP coordinates.

The rate constant for the multiphonon transitions with the energy change ΔE in a single DWP is proportional to the quantity (the number, l, of the DWP is suppressed)

$$K_{\alpha,\beta} = \frac{2\pi}{\hbar}\sum_{i,f}|\langle\Psi_f(\{\rho_j\})|\Delta(\{\rho_j\})|\Psi_i(\{\rho_j\})\rangle|^2 \frac{\exp(-\beta E_i)}{\sum_i \exp(-\beta E_i)}\delta(E_{\alpha,\beta} + E_{\mathrm{ph},i} - E_{\mathrm{ph},f}). \tag{2.5}$$

Here the initial energy $E_i = E_\alpha + E_{\mathrm{ph},i}$ contains both the initial energy of the DWP and that of the phonon subsystem, $E_{\alpha,\beta} = E_\alpha - E_\beta$. $\beta = 1/k_B T$ is the inverse temperature. It is convenient to use here the so called *non-diagonal* or *localized* representation for the DWP wavefunctions (see, e.g., Phillips 1987). They describe the 'particles' localized in one of the two wells of the DWP. They can always be chosen to be orthogonal although they are not eigenfunctions of the DWP Hamiltonian. However they have an important property that they weakly overlap exponentially in the region of the potential barrier. That is why the non-diagonal elements of the matrix $\Delta_{\alpha\beta}(\{\rho_j\})$ has the form

$$\Delta(\{\rho_j\}) = \hbar\nu\exp\{-\tfrac{1}{2}J(\{\rho_j\})\} \tag{2.6}$$

typical for the tunnelling transition amplitude where ν is a characteristic frequency. Since the quantity $J(\{\rho_j\})$ characterizing the transparency of the barrier is large for the rigid DWPs even its small fluctuations can cause strong fluctuations of the

tunnelling amplitude. A linear approximation with respect to the phonon coordinates (single-phonon approximation) would not work here and we have to make use of the multiphonon approach. The ansatz

$$J(\{\rho_j\}) = J_0 + \sum_j J'_j q_j + \tfrac{1}{2}\sum_{jj'} J''_{jj'} q_j q_{j'} \tag{2.7}$$

for the transparency parameter is assumed. Here $q_j = \rho_j - \rho_j^{(0)}$ is the deviation of the phonon coordinate ρ_j from its equilibrium value $\rho_j^{(0)}$.

The calculation described in Fleurov and Trakhtenberg (1986, see also Goldanskii *et al* 1989) results in

$$K(\pm\Delta E) = [1/\tau(T)]\exp[\pm\beta\Delta E(T)/2] \tag{2.8}$$

where

$$1/\tau(T) = (\nu^2/\Omega\sqrt{\varphi_1\varphi_2\varphi_3})\exp(-J_0 + \varphi_1) \tag{2.9}$$

and

$$\varphi_1(T) = (R/4)[\tanh(\beta\hbar\Omega/4) + R_1/2]^{-1}$$

$$\varphi_2(T) = [\sinh(\beta\hbar\Omega/4)/\cosh^3(\beta\hbar\Omega/4)]/2[\tanh(\beta\hbar\Omega/4) + R_1/2]$$

$$\varphi_3(T) = [1 + (R_1/2)\coth(\beta\hbar\Omega/4)][1 + (R_1/2)\tanh(\beta\hbar\Omega/4)].$$

The equations (2.8) and (2.9) are obtained under the assumption of the Einstein model for the oscillations of the DWP. It means that the sums over j in equation (2.7) contain only one term. It corresponds to an Einstein mode coupled with the DWP and characterized by the frequency Ω and reduced mass M. The equations (2.9) also contain two dimensionless parameters characterizing the coupling of the Enstein mode with the DWP. They are connected with the coefficients in the equation (2.7):

$$R = \hbar J'^2/2M\Omega \qquad R_1 = \hbar J''/2M\Omega.$$

Two DWP wavefunctions in the localized representation are not the eigenfunctions of the DWP. However, the latter can be obtained from the couple of localized functions with the help of the canonical transformation

$$\mathbf{T} = \frac{1}{2\Delta E}\begin{pmatrix} \sqrt{\Delta E(T) + \epsilon_a} & \sqrt{\Delta E(T) - \epsilon_a} \\ -\sqrt{\Delta E(T) - \epsilon_a} & \sqrt{\Delta E(T) + \epsilon_a} \end{pmatrix} \tag{2.10}$$

where

$$\Delta E = \sqrt{\epsilon_a^2 + \Delta_1^2(T)}.$$

ϵ_a is the asymmetry parameter of the DWP, i.e. the difference between two energies in the DWP in the *localized* representation. The coherent tunnelling amplitude $\Delta_1(T)$ is determined by the equation

$$\Delta_1(T) = \mathrm{Tr}[\varrho_{ph}(\{q_j\})\Delta(\{q_j\})]/\mathrm{Tr}[\varrho_{ph}(\{q_j\})] \tag{2.11}$$

where $\rho_{\rm ph}(\{q_j\})$ is the density matrix of the phonon subsystem. In the Einstein approximation the equation (2.11) reads

$$\Delta_1(T) = \hbar\nu^* \exp[-\tfrac{1}{2}J^*(T)] \tag{2.12}$$

where

$$\nu^* = \nu[1 + (R_1/2)\coth(\beta\hbar\Omega/2)]^{-1/2}$$

and

$$J^*(T) = J_0 - R/2[R_1 + 2\tanh(\beta\hbar\Omega/2)].$$

At low temperature the function $J^*(T)$ is a constant which determines the tunnelling amplitude renormalized due to the zero-point oscillations of the barrier. In the high temperature limit it tends to a quantity of the order of one and the next term in expansion over $1/T$ results in an activation-like behaviour with the effective activation energy $E_{\rm eff} = R\hbar\Omega/2R_1^2$. It means in particular that the Arrhenius temperature dependence of the relaxation time τ does not necessarily imply activation transitions. They can also be tunnelling in nature as well.

3. Neutron–DWP interaction

Now we start calculating the neutron scattering from the rigid DWPs using the results presented in section 2. The atoms of a glass sample interacting with neutrons are described by the Hamiltonian

$$\hat{H} = \sum_i \hat{T}_i + V(\{\boldsymbol{R}_i\}) + \sum_i W(\{\boldsymbol{r} - \boldsymbol{R}_i\}) + \hat{H}_{\rm n}. \tag{3.1}$$

It is the same Hamiltonian (2.1) in which a neutron part is added. $\hat{H}_{\rm n}$ is the Hamiltonian of the free neutrons. The interaction of a neutron with the individual atoms is described by the Fermi pseudopotential

$$W(\boldsymbol{r} - \boldsymbol{R}_i) = -2\pi\hbar^2(f_i/m)\delta(\boldsymbol{r} - \boldsymbol{R}_i) \tag{3.2}$$

where f_i is the Fermi scattering length of the ith atom, m is the neutron mass, and $\boldsymbol{r}$ is the neutron coordinate. Using the standard procedure the expression for the double-differential cross section for the neutron scattering in the Born approximation takes the form

$$\frac{{\rm d}^2\sigma}{{\rm d}\Omega{\rm d}(\delta E)} = \frac{p_f}{p_i} A v_{in} \sum_{fin} |\langle fin| \sum_i f_i {\rm e}^{-{\rm i}\kappa \boldsymbol{R}_i} |in\rangle|^2 \delta(\Delta E_{\rm g} - \delta E) \tag{3.3}$$

As usual expression (3.3) implies the summation over the final states (fin) of the glass and the statistical averaging over the equilibrium ensemble of its initial states (in). p_i and p_f are the momenta of the incident (initial) and scattered (final) neutron, respectively.

$$\delta E = {p_f}^2/2m - {p_i}^2/2m$$

is the change of the neutron energy due to its scattering, ΔE_g is the corresponding change of the glass energy including possible changes in the phonon and the DWP subsystems. $\hbar\kappa = p_f - p_i$ is the neutron momentum transfer. Equation (3.3) is the standard expression used to calculate the double-differential cross section in solids regardless of whether they are crystals or glasses. In particular, if one assumes that the bra and ket vectors in the equation (3.3) correspond to an ensemble of harmonic oscillations the standard expression for the neutron scattering by phonons arises (see, e.g., Maradudin 1966).

The initial and the final states of the glassy system will be described using the wavefunctions (2.3) in which the phonon and the DWP coordinates are separated. Assuming also that the different DWPs are spatially separated and do not interact with each other allows one to represent the DWP part of the wavefunction (2.3) as a product of the wavefunctions of the individual DWPs and the amplitude of the transitions between the DWP states for a fixed set, $\{\rho_j\}$, of the harmonic variables as the sum (e.g. (2.4))

$$\langle\psi_{\{\alpha_l\}}(\{x_l\};\{\rho_j\})|\sum_i f_i e^{i\kappa R_i}|\psi_{\{\beta_l\}}(\{x_l\};\{\rho_j\})\rangle_{\{x_l\}} = \sum_l F^{\mathrm{N}}_{l,\alpha_l\beta_l}(\{\rho_j\})\prod_{l'\neq l}\delta_{\alpha_{l'}\beta_{l'}} \tag{3.4}$$

of the individual probability amplitudes $F^{\mathrm{N}}_{l,\alpha_l\beta_l}(\{\rho_j\})$ for the transitions between the states α_l and β_l of the lth DWP. Superscript N refers to neutrons.

4. Amplitude of the multiphonon neutron–DWP scattering

Now one has to consider the $\{\rho_j\}$ dependence of the amplitude $F^{\mathrm{N}}_{l,\alpha_l\beta_l}(\{\rho_j\})$. It arises, on one hand, from the $\{\rho_j\}$ dependence of the atomic coordinates $\boldsymbol{R}_i$ in the exponential function in equation (3.4) since two sets of the coordinates are connected by the transformation (2.2). On the other hand, it is caused by the $\{\rho_j\}$ dependence of the DWP wavefunctions. We start here with the localized representation (see section 2) which is more convenient due to the exponentially small overlap of the wavefunctions belonging to different wells of the same DWP. However equation (3.3) demands eigenfunctions of the system. This will be achieved by the canonical transformation (2.10).

Relatively small momentum changes are considered here, i.e. $\kappa a_{\mathrm{DWP}} < 1$ where a_{DWP} is the characteristic scale of the DWP. This scale is believed to be close to the interatomic distance. It means that the function $e^{i\kappa R_i}$ is a slowly varying function of the coordinate x compared with the wavefunctions $\psi_\alpha(x;\{\rho_j\})$. The amplitude (3.4) for each DWP can be represented in the form

$$F^{\mathrm{N}}_{\alpha\beta}(\{\rho_j\}) = F_{\mathrm{u}}(\{\rho_j\})\delta_{\alpha\beta} + F_{\mathrm{d}}(\{\rho_j\})\sigma^z_{\alpha\beta} + F_{\mathrm{n}}(\{\rho_j\})\sigma^x_{\alpha\beta}. \tag{4.1}$$

The parameters F in the right-hand side of the equation (4.1) can be easily estimated. All three parameters can be expressed using the quantity

$$F^0 = \left|\sum_i f_i e^{-i\kappa R_i^0}\right|. \tag{4.2}$$

Here $\boldsymbol{R}_i^0$ are the equilibrium positions of the atoms associated with a given DWP. The dependence of F_u and F_d on the variation of the coordinates $\{\rho_j\}$ can be neglected which means that $F_u, F_d \approx F^0$. As for the third parameter it contains a strong exponential dependence on $\{\rho_j\}$ similarly to, e.g., (2.6),

$$F_n(\{\rho_j\}) \approx F^0 \exp\{-\tfrac{1}{2}J(\{\rho_j\})\}. \tag{4.3}$$

It is the only term in equation (4.1) contributing to the multiphonon processes. The situation is similar to that of the phonon–DWP interaction discussed in Fleurov and Trakhtenberg (1986); two types of interactions (diagonal and non-diagonal) between phonons and DWPs playing a similar role were considered there.

The matrix $\mathbf{T}$ (see equation (2.10)) transforms the matrix (4.1) written in the local representation to a new matrix in the diagonal representation:

$$\tilde{\mathbf{F}} = \mathbf{T}^{-1}\mathbf{F}\mathbf{T} = F_u\delta_{\alpha\beta} + D^d\sigma^z_{\alpha\beta} + D^n\sigma^x_{\alpha\beta} \tag{4.4}$$

where

$$D^d = ([\epsilon_a/\Delta E(T)]F_d + [\Delta_1(T)/\Delta E(T)]F_n) \tag{4.5a}$$

$$D^n = (-[\Delta_1(T)/\Delta E(T)]F_d + [\epsilon_a/\Delta E(T)]F_n). \tag{4.5b}$$

$\sigma^x_{\alpha\beta}$ and $\sigma^z_{\alpha\beta}$ are the Pauli matrices.

The term in equation (4.4) which is proportional to the unit matrix $\delta_{\alpha\beta}$ describes a motion of the DWP as a whole without changing its internal degrees of freedom. This term has nothing specific of the neutron–DWP scattering and can be attributed to the neutron–phonon scattering which is of no interest to us here. The second term proportional to $\sigma^z_{\alpha\beta}$ gives rise to the relaxation interaction. Only the terms in equations (4.5*a*) and (4.5*b*) proportional to F_n give rise to the multiphonon interaction between neutrons and DWPs. Therefore the amplitude (4.1) of the multiphonon neutron–DWP scattering after the transformation (2.10) takes the form

$$F^N_{\alpha\beta}(\{\rho_j\}) = F_n([\Delta_1(T)/\Delta E(T)]\sigma^z_{\alpha\beta} + [\epsilon_a/\Delta E(T)]\sigma^x_{\alpha\beta}) \tag{4.6}$$

which will be used in the calculations to be presented in the following section.

5. Cross section of the neutron–DWP scattering

The cross section of the multiphonon scattering of neutrons by a DWP is calculated using equation (3.3) with scattering amplitude (4.6):

$$\frac{d^2\sigma_m}{d\Omega d(\delta E)} = \frac{p_f}{p_i}Av_{in}\sum_{fin}|\langle\Psi_{fin}(\{\rho_j\})|F_n(\{\rho_j\})|\Psi_{in}(\{\rho_j\})\rangle|^2$$

$$= \{2(\Delta_1(T)/\Delta E(T))^2\delta(\Delta E_{ph} - \delta E) + (\epsilon_a/\Delta E(T))^2[f(\beta\Delta E(T))\delta(\Delta E(T) + \Delta E_{ph} - \delta E) + f(-\beta\Delta E(T))\delta(-\Delta E(T) + \Delta E_{ph} - \delta E)]\} \tag{5.1}$$

where $f(\beta\Delta E) = [1 + \exp(\beta\Delta E)]^{-1}$ gives the probability of the occupation of the upper DWP state, $f(-\beta\Delta E)$ is that for the lower state. ΔE_{ph} is the change in the

energy of the phonon subsystem. In order to get the cross section for an ensemble of the DWPs expression (5.1) should be averaged with the proper distributions of the DWP parameters.

The averaging over the initial and summation over the final states of the DWP is carried out explicitly in equation (5.1). Its first term stems from the diagonal part of the amplitude (4.6) (proportional to σ^z) and describes the elementary processes of neutron scattering in which the DWP state does not change. The remaining part is due to the non-diagonal part of the amplitude (4.6) (proportional to σ^x) and describes the processes in which the state of the ith DWP changes.

The calculation of the cross section (5.1) of the neutron DWP scattering is similar to the calculation of the rate constant $K(\Delta E)$ (see section 2) presented in Fleurov and Trakhtenberg (1986). Accounting for equation (4.3) the vector $F_n(\{\rho_j\})$ is written as

$$F_n(\{\rho_j\}) = (F^0/\hbar\nu)\Delta(\{\rho_j\}). \tag{5.2}$$

Relation (5.2) allows one easily to express the cross section (5.1) for the neutron–DWP scattering using the known equation for the rate constant $K(\pm\Delta E)$ described in section 2. The result is

$$\frac{d^2\sigma_m}{d\Omega d(\delta E)} = \frac{1}{6\pi\hbar}\left(\frac{F^0}{\nu}\right)^2 \frac{p_f}{p_i}\sum_{DWP}\frac{1}{\tau(T)}e^{-\beta\delta E/2}$$
$$\times [(\Delta_1(T)/\Delta E(T))^2 + (\epsilon_a/\Delta E(T))^2 \cosh^{-1}\tfrac{1}{2}\beta\Delta E(T)]. \tag{5.3}$$

Each individual DWP is characterized by the vector $\boldsymbol{F}_0$. Here we have neglected a possible distribution of the lengths of this vector and carried out the averaging over its orientations. The summation over DWPs in the equation (5.3) implies averaging over various values of the tunnelling parameter J_0 and over the asymmetry parameter ϵ_a. Due to the lack of any detailed information concerning these distributions this averaging presents certain difficulties. However we shall make here the same assumptions as those discussed in detail in Fleurov and Trakhtenberg (1986) where the main point was a narrow distribution of the parameter J_0 and a broad distribution of the parameter ϵ_a. It would actually mean that the temperature dependence of the cross section is not essentially changed by the averaging procedure. Therefore we may concentrate in the discussion on the results concerning the behaviour of an individual DWP.

6. Discussion

The principal result of this paper is given by equation (5.3) for the multiphonon contribution to the double-differential cross section of the neutron–DWP scattering in glasses. As mentioned in the introduction the role of a competitor can be played by the relaxation mechanism. This mechanism was discussed in Buchenau (1985) and Buchenau *et al* (1988). (Maleyev (1986) considered this mechanism in the low-temperature region.) The following equation for the relaxation double-differential cross section was obtained:

$$\frac{d^2\sigma_r}{d\Omega d(\delta E)} = \frac{2}{\pi\hbar}\frac{p_f}{p_i}\sum_{DWP} I(\Delta p)\frac{\tau}{(\delta E\tau/\hbar)^2+1}\cosh^{-2}(\beta\Delta E/2) \tag{6.1}$$

where $I(\Delta p)$ is a factor similar to that in equation (4.1) and connected with the geometry of the DWP. Comparing two cross sections (5.3) and (6.1) one can roughly estimate their ratio as

$$[\mathrm{d}^2\sigma_\mathrm{m}/\mathrm{d}\Omega\mathrm{d}(\delta E)]/[\mathrm{d}^2\sigma_\mathrm{r}/\mathrm{d}\Omega\mathrm{d}(\delta E)] \simeq \mathrm{e}^{-\beta\delta E/2}[1+(\tau\delta E/\hbar)^2]/(\tau\nu)^2. \tag{6.2}$$

The answer to the question which mechanism, the relaxation or the multiphonon, is dominant depends on the value of two dimensionless quantities: $\beta\delta E$ and $\tau\delta E/\hbar$. In the usual experimental situation $1/\tau(T)$ does not exceed a few GHz while $1/\beta h = 20T$ GHz where T is the temperature measured in Kelvins. It means that the exponential function in equation (6.2) changes more slowly than the Lorentzian function coming from the relaxation cross section. Therefore there is a range of the transfer energies, δE, and temperatures where we are beyond the maximum of the Lorentzian ($\tau\delta E \gg 1$) whereas the exponential factor has not yet decayed ($\beta\delta E \ll 1$). In this range the multiphonon mechanism is predominant. This situation is similar to that discussed in Fleurov and Trakhtenberg (1986) for the DWP–phonon scattering.

The construction of equation (5.3) is simple so that various dependencies do not interfere. For example, the dependence of the cross section on the change, κ of the neutron wavevector, i.e. the form factor, is not practically influenced by the temperature and the transfer energy changes. This type of behaviour was emphasized by Buchenau *et al* (1984).

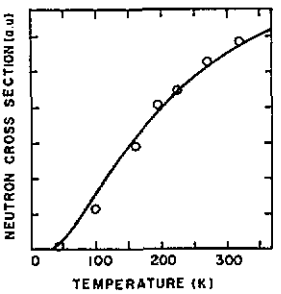

Figure 1. The temperature dependence of the cross section for the multiphonon neutron–DWP scattering for the neutron transfer energy, 220 GHz. The circles show the experimental data of Buchenau *et al* (1988). The theoretical results are shown by the full curve.

As for the temperature dependence of the multiphonon cross section it differs essentially from that of the relaxation one. Really the relaxation cross section has a maximum as a function of the temperature in the region determined by the equation $\tau(T)\delta E/\hbar = 1$ while for the multiphon cross section this condition is of no importance. Its temperature dependence is determined mainly by the temperature dependence of the factor $1/\tau(T)$ in the equation (5.3) which is monotonic. Equation (2.9) gives us a simple expression for the relaxation time $1/\tau(T)$ in the multiphonon regime which can be used in order to compare the theoretical results with the experimental ones (see figure 1). The parameters $R = 500$, $R_1 = 4.5$ are chosen to fit the data of Buchenau *et al* (1988). The frequency $\Omega/2\pi$ of the local mode coupled with the DWP is chosen to be 0.64 THz. These values are close to the parameters used in Fleurov and Trakhtenberg (1986) for DWP–phonon scattering. The most important point here is that now we have no problems with the maximum which is inevitable in the relaxation mechanism but is absent both in the experiment and in the theory proposed in this paper on the basis of the multiphonon mechanism. This fact together with the other features of the multiphonon cross section mentioned earlier allows us to hope that this mechanism plays an essential role under the conditions of the current experiments.

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