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# PHONON DENSITY OF STATES AND COHERENT INELASTIC NEUTRON SCATTERING ON COMPLEX STRUCTURES

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Плотность фононных состояний и когерентное рассеяние нейтронов на сложных структурах

Исходя из метода псевдопотенциалов описывается метод расчета фононного спектра для когерентно рассеивающихся веществ сложных структур. Для $MgZn_2$ в качестве примера сравниваются теоретические и экспериментальные результаты. Получено хорошее согласие.

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Phonon Density of States and Coherent Inelastic Neutron Scattering on Complex Structures

Model potential calculations for $MgZn_2$ were used to get the corresponding spectrum of neutrons inelastically scattered by $MgZn_2$. A good agreement between the calculated and measured neutron spectra was found.

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Neutron inelastic scattering has been proved to be an excellent tool for investigating phonon dispersion relations in crystals. In the case of complex structures with many atoms in the unit cell, however, a direct determination of the phonon density of states or some related quantity might be a more proper experimental approach in several aspects. For incoherent scatterers the phonon density of states $g(\omega)$ may be immediately obtained from neutron scattering on polycrystalline samples. Unfortunately most substances are rather poor incoherent scatterers. Therefore, an effort has been made to extract the phonon density of states from the intensity of coherent inelastic neutron scattering on polycrystalline samples by means of some extrapolation procedures (see e.g. /1/) or by means of special experimental equipment first discussed by Oskotski et al. /2,3,4/. The idea is the following. The structure factor

$$F_s(\vec{q}) = \left| \sum_i \frac{a_{i,\,cob}}{\bar{a}'_{cob}} \cdot e^{-W_i(\vec{K})} e^{i\vec{K}\vec{R}_i} \frac{\kappa \cdot \vec{e}_i(s,\vec{q})}{\sqrt{M_i}} \right|^2, \quad (1)$$

which occurs in the expression for the coherent cross section of a single crystal

$$\frac{d^2\sigma}{d\Omega\, dE} = \frac{\hbar}{2}\frac{k}{k_0}\bar{a}'^2_{cob} \sum_s \int d\vec{q}\, \delta(\vec{\kappa}-(\vec{q}-\vec{K}))\frac{n_{s,\vec{q}}+1}{\omega_{s,\vec{q}}} \times \delta(\epsilon-\hbar\omega_{s,\vec{q}}) \cdot F_s(\vec{q}), \quad (2)$$

depends on the phonon polarization $s$ and wave vector $\vec{q}$. In (1) and (2) $a'_{i,coh}$ is the coherent scattering length of the nucleus at site $\vec{R}_i$ in the unit cell, $M_i$ is the mass of this nucleus and $\vec{e}_i(s,\vec{q})$ is its polarization vector, $exp(-W_i(\vec{\kappa}))$ is the Debye-Waller factor, $k_0$ and $k$ are the momentum of the incident and scattered neutron, $\epsilon$ and $\vec{\kappa}$ are the energy and momentum transfer of the neutron, respectively; $\bar{a}'_{coh}$ is the coherent scattering length, averaged over the unit cell, $n_{s,\vec{q}}$ is the phonon occupation number, $\omega$ is the phonon frequency, and $\vec{K}$ is a reciprocal lattice vector. If the coherent cross section (2) is averaged over all directions (polycrystalline samples) and over many Brillouine zones - so that the structure factor (1) is averaged to a constant - we obtain from (2) direct information on the phonon density of states. Unfortunately the average over many Brillouine zones may often be achieved only by forcing the neutrons to a twofold scattering process (elastic and inelastic) /3/. Consequently, a price in intensity is paid. But even in this case some assumption for isotropic distributed polarization vectors has to be made, which is only known to be well realized in cubic structures /2/.

Therefore, a direct check of the theoretical model by means of coherent inelastic neutron scattering on polycrystalline samples requires in many cases a calculation of the intensity of scattered neutrons as a function of the energy transfer using (2) and taking into account experimental conditions. This function may be folded with the energy resolution function of the spectrometer in order to give a quantity, which immediately corresponds to the measured neutron intensity. Thus we have a situation similar to that in the case of soft $X$-ray spectroscopy of electronic states in a crystal, where the comparison of experiments with band stracture calculations requires the calculation of the $X$-ray spectra by means of wave functions and energies of the band structure calculation (see e.g. /5/).

In a previous paper /6/ the phonon spectra of the intermetallic compound $MgZn_2$ were investigated theoretically and experimentally, and rather interesting features connected with a soft mode behaviour were found in the calculation. We, therefore, were much interested in a reliable comparison between theory and experiment to check the model used in the calculations. In /6/ we assumed that the conditions for Oskotski's treatment were approximately fulfilled in the experiment. On this basis the calculated phonon density of states was compared with the experimental curves. Later we calculated the structure factor (1), averaged in a way corresponding to the experimental conditions, and found that our assumption ($F_s(q) \approx const.$) was only rather a poor approximation. Therefore, we followed the procedure outlined above and calculated the neutron spectrum from the phonon frequencies $\omega_{s,\vec{q}}$ and polarization vectors $\vec{e}_i(s,\vec{q})$.

The results are given in Fig. 1. It may be seen that the calculated neutron spectrum (a) folded with the resolution function of the spectrometer gives (b) and has the same general behaviour as the experimental curves (c) as it was found in Fig. 9 of /6/. The measured cut-off frequency 1 and the maxima 2,3,4 are shifted to lower frequencies, which indicates an error for the calculated cut-off frequency of about 20%. Taking into accout that the calculations /6/ do not involve any fitted parameter, the agreement between experimental and theory is good. A comparison between the calculated neutron spectrum (b) and the phonon density of states (a) shows, that the maxima 2,3,4 in the neutron spectrum come from peaks in the density of states. It seems to us that this circumstance makes the neutron spectrum usefull for a rough determination of the phonon density of states in those cases too where the conditions for the Oskotski's treatment are not fulfilled.


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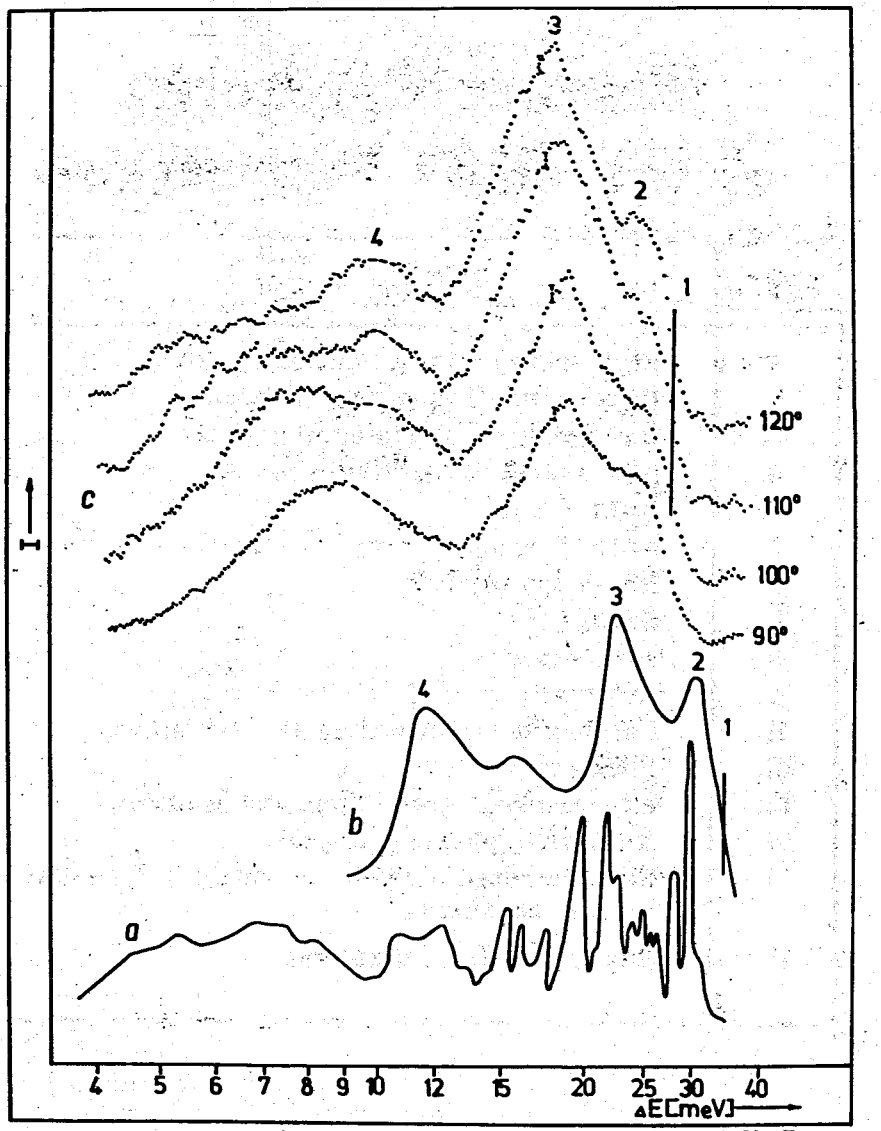


a) Calculated phonon density of states $g(\omega)$ of $MgZn_2$. b) Calculated neutron spectrum for a polycrystalline sample of $MgZn_2$ at the scattering angle 100° folded with the resolution function of the spectrometer. c) Measured neutron spectrum of inelastically scatered neutrons on $MgZn_2$ at 300K and different angles 90° , 100° , 110° , 120° .