FİZİKA 2008 CILD XIII №3

LATTICE DYNAMICS OF $TlInSe_2$ STUDIED BY INELASTIC NEUTRON SCATTERING

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İlk dəfə olaraq $TlInSe_2$-in neytronografik tədqiqi aparılmışdır. Göstərilmişdir ki, $TlInSe_2$-də istilik neytronlarının qeyri-elastiki səpilməsinin, İn atomlarının səpilmə kəsiyinin olduqca kiçik olmasına baxmayaraq, xətası 5 meV-u aşmayan fonon tezliklərini və onların dispersiyasını təyin etməyə imkan verir.

Проведены первые нейтронографические исследования $TlInSe_2$. Показано, что неупругое рассеяние тепловых нейтронов позволяет с точностью не менее 5 meV определить частоты фононов и их дисперсию в $TlInSe_2$, несмотря на довольно малое сечение рассеяния атомами In.

The first neutronographic studies of $TlInSe_2$ have been performed. It is shown that inelastic scattering of thermal neutrons allows to obtaining phonon frequency and dispersion with an accuracy higher than 5 meV in spite of the rather small scattering cross sections of In atoms.

Ternary Tl-compounds with TlSe-type structure attract strong attention because of their large thermoelectric power. $TlInSe_2$, with a figure of merit for thermoelectric performance above 3, is foreseen as a member of a new class of thermoelectric materials [1].

$TlInSe_2$ has a tetragonal layer-chain structure (space group $I4/mcm$, a=8.075Å and c=6.847 Å at 300 K) [2], which can be formally described as a set of $(In^{3+}Se^{2-})^-$ chains extended along the *c*-axis and connected with each other through monovalent Tl^+ ions. It is assumed that structural one-dimensionality of the material leads to one-dimensionality of the phonon spectra and is, ultimately, behind the huge thermoelectric power of $TlInSe_2$. Understanding the thermoelectric properties through extendig and developing the knowledge of physical properties of $TlInSe_2$ is very important.

The aim of the experiment was to demonstrate the feasibility to investigate the phonon dispersion of $TlInSe_2$ by inelastic neutron scattering in spite of the small scattering cross-sections of the İn atoms. The basis of the experiment was the newly calculated dispersion relation of $TlInSe_2$ (figure 2).

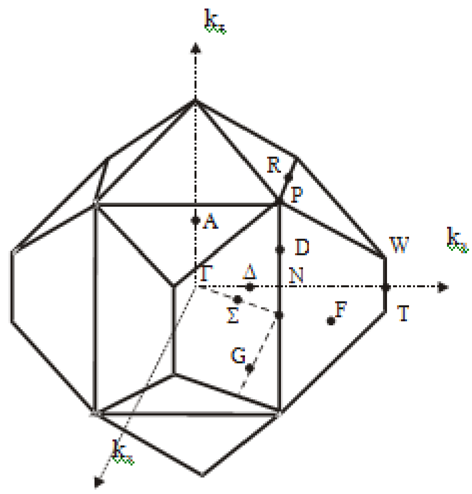

Figure 1: The Brillouin zone with the notation of symmetry points and lines. The point T has the coordinates (0, 2π /a, 0), the point N the coordinates (π /a, π /a, 0).

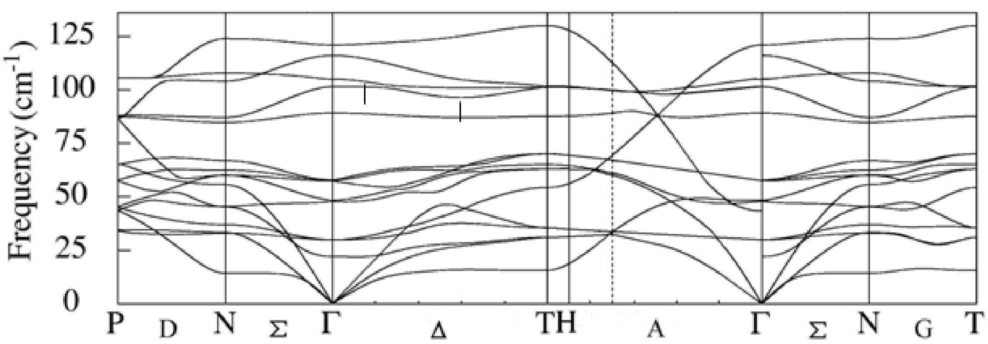

Figure 2: Calculated phonon dispersion in $TlInSe_2$ in a region up to 125 cm^{-1}. The point T has the coordinates (0, 2π /a, 0). The phonon energies are given in cm^{-1}(100 cm^{-1} =12.4 meV).

Inelastic neutron scattering experiments were carried out at the triple axis spectrometer for thermal neutrons at constant $\mathbf{k}_i$ using incident energies of E_i=14.2 meV and 53.378 meV, respectively. The horizontal collimation was 80'-40'-40'-40'. Different constant-**q** scans with q=0.1 $Å^{-1}$ and 0.5 $Å^{-1}$ were performed in the [010] direction, i. e. between the Γ-point and T (see marked regions in figure 2). Within the energy transfer range studied with E_i=53.378 meV, figure 3 shows one scan for example, the results indicate a flat phonon dispersion in agreement with the model calculations.

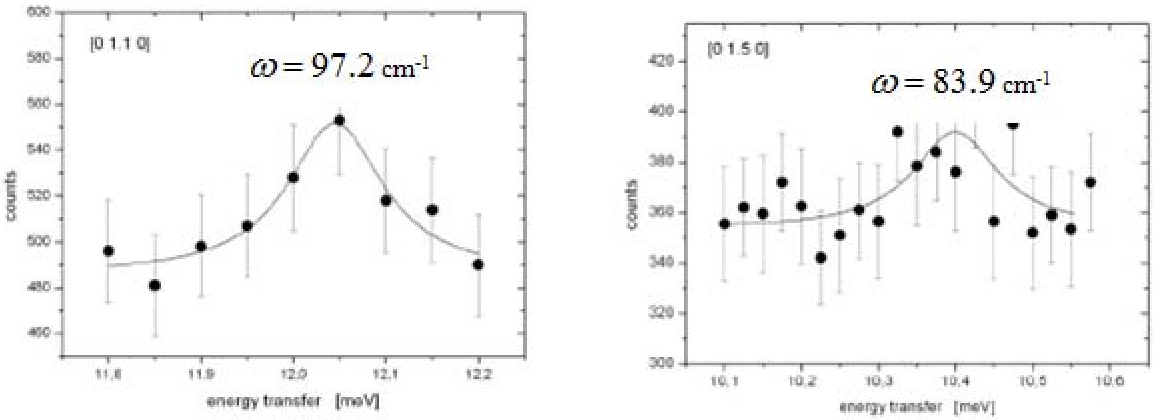

Figure 3: Constant-**q** scan in [010] (i. e. between the Γ-point and T in figure 2) with q=0.1 $Å^{-1}$ (left) and q=0.5 $Å^{-1}$ (right). The solid line corresponds to a fit using a Lorentzian line shape.

[1]. *N. Mamedov et al.,* Thin Sol. Films 499 (2006) 275.

[2]. *D. Müller, G. Eulenberg, H. Hahn,* Z. anorg. Allg. Chem. 398 (1973) 207.