INVESTIGATION OF THE QUASILOCAL LEVEL IN THE VIBRATION SPECTRUM OF A LATTICE WITH HEAVY IMPURITY ATOMS

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The distortion of the phonon spectrum of a metal (Mg) as a result of introduction of a heavy impurity atom (2.8% Pb) was investigated experimentally. Inelastic scattering of cold neutrons was used. The data are in satisfactory agreement with the theoretical predictions of Kagan and Iosilevskiĭ.[1]

IN a paper of Kagan and Iosilevskiĭ[1] it was pointed out that the vibration spectrum of a heavy impurity atom of mass m' in a lattice of light atoms of mass m, when $m'/m \gg 1$, has a markedly resonant character. The singularity of the vibration spectrum is localized near a frequency ω_0:

$$\omega_0 = \omega_{max}[|1 - m'/m| \times \langle(\omega/\omega_{max})^{-2}\rangle]^{-1/2}, \qquad (1)$$

where ω_{max} is the limiting frequency for the lattice without the impurity. Later this point was also noted in other papers.[2,3] Obviously such a change in the phonon spectrum of a crystal containing a heavy atom as compared to the spectrum of the initial crystal will cause marked changes in the thermodynamic[4] and kinetic[5] properties. But until now there have been no direct experimental confirmations of the theoretically predicted changes in the phonon spectrum of a crystal with a heavy impurity atom.

We have attempted to observe the quasilocal level in the vibration spectrum of a lattice with a heavy impurity atom by using inelastic scattering of neutrons. The detailed theory of the inelastic scattering of neutrons by a crystal containing impurity atoms was developed in [6].

We investigated a solid solution of Pb and Mg containing about 2.8 at% Pb. This alloy is very suitable for study by means of neutrons since: (1) the mass ratio is large ($m'/m = 8.5$), so that we may expect that the quasilocal level will be located in a region where the density of states is low, and (2) the absorption cross section is small for both components of the alloy and the difference in their neutron scattering cross sections is large.

Measurements of inelastic scattering of cold neutrons by polycrystalline samples of pure Mg and the alloy $Mg_{0.972}Pb_{0.028}$ were made on a time-of-flight spectrometer. The neutron transmission of the sample for the primary line was 0.92. The measurements were carried out at room temperature. The number of Mg atoms was the same in both samples.

The initial data of the measurements of spectra of inelastically scattered neutrons as a function of neutron wave length λ_n are presented in Fig. 1. The data were corrected for background and normalized to the same incident flux. As we see from the figure, in the region of large λ_n (small energy changes) the spectrum of the neutrons scattered from the sample of the solid solution of $Mg_{0.972}Pb_{0.028}$ goes much higher than that for pure Mg.

In Fig. 2 we give the experimental data on the energy dependence of the ratio of the intensity $N'(\Delta E)$ of neutrons scattered by the alloy $Mg_{0.972}Pb_{0.028}$ to the intensity $N(\Delta E)$ scattered by Mg. Since the measurements were done under completely identical conditions, this ratio represents the ratio of the inelastic scattering cross

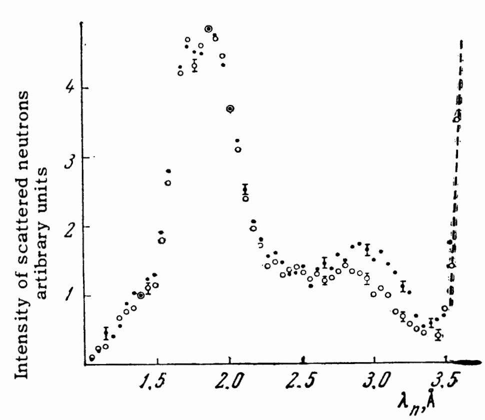

FIG. 1. Spectrum of neutrons inelastically scattered from $Mg_{0.972}Pb_{0.028}$ (solid points) and Mg (open circles). The dashed line shows the start of the elastic scattering region.

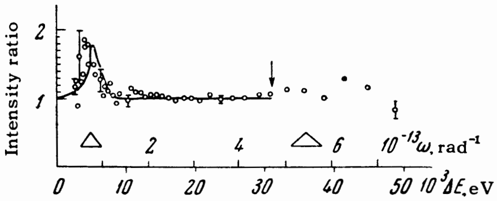

FIG. 2. Ratio of cross section for neutron scattering by $Mg_{0.972}Pb_{0.028}$ to cross section for scattering by Mg: points-experiment, curve-calculation. The arrow indicates the limit of the Mg phonon spectrum.

sections, taken per atom of Mg. At low energy transfers (low frequencies) this ratio has a sharp maximum, which is related to the fact that in the low energy region the cross section for inelastic scattering by the crystal containing a heavy impurity atom increases rapidly.

Obviously this cross section ratio can be written as

$$N'(\Delta E)\,/\,N(\Delta E) = 1 + AF(\omega), \quad (2)$$

where A is a constant which is determined by the impurity concentration and the ratio of the neutron scattering cross sections of the impurity atom and the atom of the initial lattice. The function $F(\omega)$ is connected with the contribution to the phonon spectrum of the quasilocal level; under ideal resolution, according to [6], it is proportional to the spectral density of vibrations of the impurity atom. This function can be calculated easily for any specific form of the vibration spectrum of the host crystal. The computational results, done on a Debye model for Mg, are shown in Fig. 2 by the solid curve.

One's attention is drawn to the fact that both the energy and width of the maximum in the cross section ratio show satisfactory agreement of theory and experiment. The possibility is not excluded that the observed local level has a fine structure, since two quasilocal levels should be split off in the hexagonal Mg lattice. However, because of poor resolution of the equipment in the low energy region, one is unable to resolve the fine structure of the level. Further measurements with better resolution and better statistics are needed.

Thus, as a result of studying the inelastic scattering of cold neutrons by samples of solid solution $Mg_{0.972}Pg_{0.028}$ and pure Mg, we have shown that small admixtures of heavy impurity atoms in the lattice of light atoms drastically change the phonon spectrum of the crystal in the low frequency region, resulting in the appearance of quasilocal vibrations.

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