

STATE DENSITY OF PHONONS IN CADMIUM

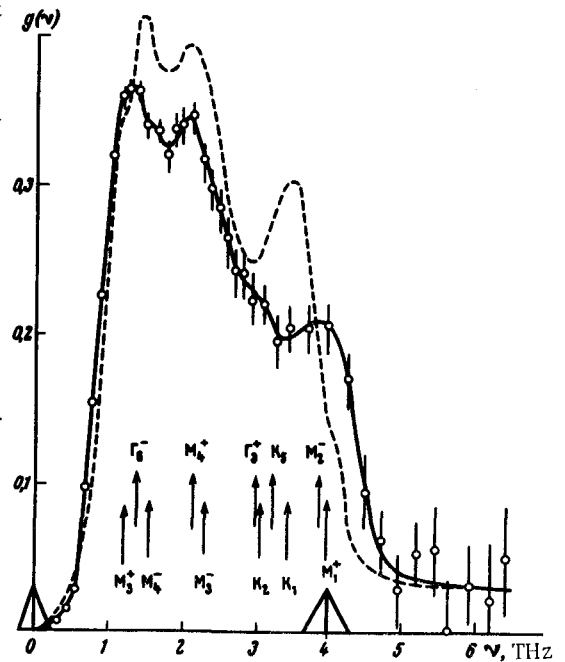
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Using inelastic neutron scattering, we determined the density $g(\omega)$ of the phonon states in cadmium. The measurements were performed on a mixture of the isotopes Cd-110 and Cd-111. The density of states was obtained by integrating the cross section for scattering by a polycrystal in a wide range of momentum transfers. Using the analogy between $g(\omega)$ of Cd and Zn, we determined the frequencies of the phonons in cadmium for certain symmetric points of the Brillouin zone.

In recent years, considerable progress was made in the microscopic description of the electronic and atomic properties of simple transition metals (alkali metals, Mg, Al), including the phonon spectrum. In the case of more complicated metals with filled d- and f-bands, fundamental difficulties arise. On the one hand, these difficulties are connected with the more complicated forms of the initial pseudopotentials, which are essentially nonlocal in nature and contain in a number of cases a resonant dependence on the electron energy [1]. On the other hand, the difficulties are due to need for taking into account higher-order perturbation theory terms in the calculation of the band-structure energy [2]. These questions, which are important for the microscopic theory of metals, can be explained to a considerable degree by investigating the phonon spectra of Zn and Cd, which are strongly anisotropic hexagonal crystals ($c/a = 1.856$ and 1.886 , respectively) and whose d-bands are either close to the conduction band or partly overlap it [3].

Unlike Zn, which has been investigated in sufficient detail [4, 5], the information on the phonon spectrum of Cd is limited only to results [6] obtained by the method of diffuse scattering of x-rays, which is of limited accuracy. Cd was not investigated before with the aid of neutron scattering, owing to the large absorption at thermal energies. At the first stage in the study of the phonons in Cd, we determined the density of stages $g(\nu)$ by a method developed for coherently scattering crystals of arbitrary symmetry in [7, 8] under the influence of the results of [9]. The method used data on the neutron scattering law $S_{coh}(\kappa, \epsilon)$, measured in a wide range of momentum transfers κ and energies ϵ . The experimental technique and the procedure for determining $S_{coh}(\kappa, \epsilon)$ are described in [8, 10].

The work was performed on polycrystalline samples of the separated isotopes Cd-110 and Cd-111 (~ 280 g), additionally rid of the strongly absorbed Cd-113 by bombardment with a flux $\sim 10^{20}$ neut/cm² in the MR reactor of our Institute. As a result, the Cd-113 content was decreased to 10^{-4} ($\sigma_T^1 < 2.0$ b). The chemical purity of the samples was determined by the content of the light-element impurities, which did not exceed 2×10^{-4} . The measurements were performed on a "thin" sample ($\Sigma d \approx 0.130$) at $T = 290^\circ\text{K}$ at incident neutron energies $E_0 = 18.5, 20.9, \text{ and } 21.8$ meV with resolution $\Delta E = 0.8 - 0.9$ meV and for 24 scattering angles from 24 to 116° . These conditions ensured a sufficiently homogeneous and dense distribution of the κ vectors in a large volume of reciprocal space (~ 200 Brillouin zones), and made it possible to trace the transition to the incoherent approximation when the region of integration of the single-phonon cross sections $S_{coh}^1(\kappa, \epsilon)$ with respect



Phonon spectrum of Cd reconstructed from $S_{coh}^1(\chi, \epsilon)$ at $E_0 = 21.8$ meV. The triangles show schematically the ϵ -dependent resolution function of the spectrometer, and the dashed line shows the "reduced" spectrum of Zn.

to was expanded. The procedure for reconstructing $g(\nu)$ and estimating the resultant errors is given in [7, 8].

The phonon state density in Cd is shown in the figure. Since the isotropic effect in Cd is less than one per cent, we can consider $g(\nu)$ to be obtained for the natural isotope mixture. The Cd spectrum is characterized by a narrow Debye region limited to ~ 0.5 THz, and by a large density of the low-frequency states. This character of $g(\nu)$ is connected with the anisotropy of the Cd lattice, since the splitting of the branches of the transverse acoustic oscillations in the Σ and T directions is accompanied by a decrease in the frequencies of the phonons with polarization along the c axis (the branches Σ_3 and T_3), which leads to a strong singularity at $\nu \sim 1.3$ THz. This tendency was observed earlier in Zn [5] and is probably even stronger in Hg [11].

The phonon spectrum of Cd turned out to be quite similar to the Zn spectrum. This is seen from the figure, in which $g(\nu)$ of Zn is constructed with allowance for the ratio of the ion plasma frequencies $\sqrt{(MV)_{Cd}/(MV)_{Zn}}$ (M is the mass of the nucleus and V is the unit-cell volume); the singular-point frequencies determined in [4] were noted. The maximum differences occur in the region of the frequencies of the longitudinally-polarized oscillations ($\nu > 3.0$ THz), which are most sensitive to the character of the pseudopotential and to details of the electron-electron interaction. Near the end point of the spectrum in Cd, a considerable increase of the density of states is observed at a relatively fair agreement between the position of the last singularity with the "reduced" end-point frequencies of the longitudinal Σ branches of Zn (the points M_1^+ and M_2^+). This may be connected with the difference between the behavior of the T branches near the end of the band, particularly with the relative increase of the frequency of the longitudinal optical phonons at the point K_1 . On the basis of these considerations we identified the main singularities of $g(\nu)$ of Cd and estimated the phonon frequencies in the following points of the band (see the table).

The values of the frequencies at the points M_1^+ and M_2^+ differ strongly from the data of [6], which are listed in the lower line of the table. The obtained frequencies can be used to determine the parameters of the model potential [1] and in the calculation of the phonon spectrum [12].

The function $g(\nu)$ shown in the figure describes well the thermodynamic properties of Cd: the calculated specific heat, the rms atom displacements, and the corresponding Debye temperatures agree with calorimetric and x-ray measurement data in a wide temperature range [5].

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Direction	Δ		T			
	Δ_2, LO	Δ_6, TO	T_1, LO	$T_1, LA; T_4, TO \perp$	$T_4, TA \perp$	$T_2, TO \parallel; T_3, TA \parallel$
Point	Γ_3^+	Γ_6^-	K_1	K_5	K_2	K_6
Frequency, THz	3.0 ± 0.2	1.4 ± 0.15	3.6 ± 0.25	3.25 ± 0.2	3.1 ± 0.2	1.1 ± 0.1
	2.9	1.5	-	-	-	1.3
Direction	Σ					
Branch	Σ_1, LO	Σ_1, LA	$\Sigma_4, TO \perp$	$\Sigma_4, TA \perp$	$\Sigma_3, TO \parallel$	$\Sigma_3, TA \parallel$
Point	M_1^+	M_2^-	M_3^-	M_4^+	M_4^-	M_3^+
Frequency, THz	4.1 ± 0.25	3.9 ± 0.25	2.4 ± 0.2	2.2 ± 0.2	1.6 ± 0.15	1.3 ± 0.15
	6.4	5.1	2.5	2.4	1.8	1.3

(\parallel — phonon polarization along the c axis, \perp — in the (0001) plane).

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SINGULARITIES OF THE SPECIFIC HEAT OF FERRITES IN A MAGNETIC FIELD IN THE VICINITY OF THE CURIE POINT

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Experimental data are presented on the specific heat of the ferrite $\text{Cu}_{0.4}\text{Cd}_{0.6}\text{Fe}_2\text{O}_4$ in the vicinity of the phase transition, as a function of the external magnetic field intensity. The H-T phase diagram of the ferrite near the Curie point is obtained from these measurements. A discussion of the results is presented.

The main purpose of studying critical phenomena, namely to establish the exact form of the singularities of the physical parameters, including the specific heat (C), has not yet been attained. The only reliably known fact is that the character of the singularity of the specific heat in the critical region does not agree with the Weiss-Van der Waals-Bragg theory. There are even fewer studies of the behavior of the specific heat if the external conditions are altered. We present here the results of an investigation of the specific heat of $\text{Cu}_{0.4}\text{Cd}_{0.6}\text{Fe}_2\text{O}_4$ in the vicinity of the Curie point T_c . From the magnetic point of view, this ferrite is ferrimagnetic with three magnetic sublattices. The complicated magnetic sublattice structure may affect the behavior of C, particularly if it is investigated in a magnetic field H. The character of the anomalies of the specific heat at T_c of ferrites in an external field has not been investigated so far. The measured values of C of $\text{Cu}_{0.4}\text{Cd}_{0.6}\text{Fe}_2\text{O}_4$ in fields $H = 0, 0.14, 4.2, 8.3, 13.2,$ and 20.2 kOe are shown in Figs. a and b.

