
修士論文アブストラクト

(1981 年度)

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1. Study on Lattice Dynamics of Layered Structure CoCl_2
by Raman scattering

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ABSTRACT

The single crystal of CoCl_2 has the CdCl_2 structure, which is a typical layered structure. The layers are perpendicular to the crystallographic c -axis. The metal ions and the halogen ions are bonded by the mixed-covalent-ion bonding, which displays a halogen-metal-halogen sandwich-layer structure. The inter=layer-interaction is very weak compared with the intra-layer=interaction. So the anisotropic lattice vibration is expected to be observed. In this report, the anisotropy of the lattice dynamics of CoCl_2 has been studied by the Raman spectroscopy.

The CoCl_2 crystal has two Raman active modes. One is A_{1g} mode caused by the compressional forces between Co-sheets and Cl-sheets. The other is E_g mode caused by the shearing forces between them. The spectral frequencies, widths and intensities of these two modes

have been investigated over the temperature range of 22K-573K. In order to clarify the anisotropy on the propagating direction of phonons, two experimental geometries, ($q\parallel c$ -axis) and ($q\perp c$ -axis), have been used. Thus the Raman spectra of the following four modes have been obtained; $A_{1g}(L)$ ($q\parallel c$ -axis), $E_g(T)$ ($q\parallel c$ -axis), $A_{1g}(T)$ ($q\perp c$ -axis) and $E_g(L+T)$ ($q\perp c$ -axis).

It is well known that the change of the spectral widths and frequencies with the temperature change are caused by the anharmonic terms of the interatomic interactions. The experimental results of the temperature dependence of the spectral widths and frequencies indicate following points. (1) The temperature dependence of both spectral widths and frequency shifts of E_g mode are larger than those of A_{1g} mode. So the contribution of the anharmonic terms on the E_g mode is more than that on the A_{1g} mode. (2) The temperature dependence of both the spectral widths and frequencies of A_{1g} mode decreases at 300K-400K. So the contribution of the anharmonic terms on the A_{1g} mode decreases at 300K-400K.

The temperature dependence of the spectral intensities of these modes indicate following points. (3) As the temperature increases, the intensities of both $A_{1g}(L)$ and $E_g(T)$ modes which propagate along the c -axis do not increase as expected by the spectral formula. This deviation is explained by the disappearance of the long range correlation along the c -axis. (4) As for $A_{1g}(T)$ and $E_g(L+T)$ modes which propagate in the c -plane, the intensities of these two modes increase according to the spectral formula as the temperature increases to 300K-400K. (5) In the temperature range of $T \gtrsim 300\text{K}-400\text{K}$, the intensity of $A_{1g}(T)$ mode decreases rapidly, which relates to (2), the behavior of A_{1g} mode. These phenomena indicate that the interactions in the c -plane between the Cl-atoms become to vanish above room temperature. (6) In the temperature range of $T \gtrsim 300\text{K}-400\text{K}$, the spectral intensity of the $E_g(L+T)$ mode does not decrease so rapidly as that of the $A_{1g}(T)$ mode. This is consistent with the result of the Mössbauer measurement, in which the mean square values of the displacements perpendicular to the c -axis does not increase at $T \gtrsim 300\text{K}-400\text{K}$. These behavior of the $E_g(L+T)$ mode indicate the solidity of the Cl-Co-Cl layer in the c -plane, which is the typical character of the CdCl_2 structure.

The present results mentioned above give the microscopic picture toward melting and sublimation of this type of material.