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INVESTIGATION OF THE CHARGE DENSITY WAVES IN 2H-TaSe₂ BY ONE AND TWO PHONON RAMAN SCATTERING

S. Sugai**, K. Murase*, S. Uchida** and S. Tanaka**

*Department of Physics, Osaka University, Toyonaka, 560 Japan
**Department of Applied Physics, University of Tokyo, Tokyo, 113 Japan

Abstract. - One and two phonon Raman scattering was investigated in 2H-TaSe₂ at the normal and the charge density wave (CDW) phases. The temperature dependence of the generalized susceptibility was obtained from the integrated scattering intensity of the two phonon peaks relating to the Kohn anomaly mode. The temperature dependence of the phonon energies calculated from this susceptibility shows excellent agreement with the experimental data obtained from one phonon Raman scattering in the soft A₁g and E₂g - modes in the CDW phase and the Kohn anomaly mode in the normal phase.

Transition metal dichalcogenide 2H-TaSe₂ is a typical layered compound with a CDW phase transition. The crystal structure changes from the original hexagonal phase D₆h to the incommensurate charge density wave (CDW) phase at 122 K, followed by the triply commensurate CDW (TCCDW) phase of 3a₀ x 3a₀ x c₀ at 90 K.¹ On warming only the stripe domain structure (SCCDW), in which one CDW is commensurate and the other two are incommensurate, was observed by x-ray diffraction between 90 K to 112 K.²

The experiment was made in the back scattering configuration on the layer plane with 5145 Å Ar-ion laser and micro-computer associated system. Using this experimental configuration, one A₁g and two E₂g modes are observed in the normal phase. In the TCCDW phase six points on the Γ-lines and the two K-points in the original phase are folded into the Γ-point.
Figure 1 shows the Raman spectra below 100 cm\(^{-1}\). The \(A_{1g}\)-spectra were obtained by subtracting the perpendicularly polarized spectra \(Z(\text{XY})\) from the parallel polarized spectra \(Z(\text{XX})\). The normalized intensity was obtained by dividing the experimentally obtained intensity by \(n + 1\), where \(n\) is the Bose-Einstein factor. The small peak at 24 cm\(^{-1}\) in the \(E_{2g}\)-spectra is due to the natively active rigid layer mode. The broad peak at 110 cm\(^{-1}\) is due to the two phonon process. On decreasing the temperature, two \(A_{1g}\)-modes and four \(E_{2g}\)-modes become strong. Figure 2 shows the temperature dependent phonon energies of these modes. The \(A_{1g}\)-mode at 82 cm\(^{-1}\) and the \(E_{2g}\)-mode at 50 cm\(^{-1}\) at low temperatures, show softening toward the CDW to the normal phase transition temperature at 122 K. The 50 cm\(^{-1}\) mode is overdamped above 110 K. The 82 cm\(^{-1}\) \(A_{1g}\)-mode approaches the 42 cm\(^{-1}\) \(A_{1g}\)-mode and merges at 100 K.

The strong two phonon scattering intensity relating to the Kohn anomaly is the distinctive feature of 2H-compounds with CDW phase transitions. The maximum position and the edge of the foot of the two phonon scattering peaks are shown in Fig. 3. The energy of the edge shows strong temperature dependence. The half of this energy corresponds to the energy of the Kohn anomaly \(\Sigma_{1}\) \(\underline{\text{A}}\)-mode. The integrated scattering intensity increases with decreasing temperature, if the intensity is normalized by the statistical factor of the two phonon emitting process. The two phonon scattering intensity is related to the generalized electronic susceptibility \(\chi_{q\lambda}^{(4)}\) by
\[
I \propto \chi_{q\lambda}^{(4)}(n + 1)^2.
\]
Figure 4 shows the obtained susceptibility. Phonon energies renormalized by the electron-phonon interaction are expressed\(^{(5)}\) by

\[
\tilde{\omega}_q^2 = \omega_{q\lambda}^2 - \alpha_{q\lambda} \chi_{q\lambda},
\]

where \(\tilde{\omega}_q^2\) and \(\omega_{q\lambda}\) are the renormalized and bare phonon frequency, respectively. The calculated phonon energies are shown in Fig. 2 and Fig. 3 by dotted curves. The agreement with the experimental results is excellent.

Our results are summarized in the following.

1. The generalized electronic susceptibility was obtained from the second order Raman scattering intensity. The energy of the Kohn anomaly mode was calculated above and below the CDW phase transition temperature using the susceptibility. The agreement with the experimental data was excellent.

2. In the CDW phase, the \(A_{1g}\)-mode at 82 cm\(^{-1}\) at 12 K and the \(E_{2g}\)-mode at 50 cm\(^{-1}\) shows strong softening and their intensity curves have shoulders at about 90 K. They might be assigned to the amplitude modes. The 42 cm\(^{-1}\) \(A_{1g}\)-mode and the 64 cm\(^{-1}\) \(E_{2g}\)-mode might be assigned to the phase modes.

3. No hysteresis was observed in the phonon energy, scattering intensity and line width in the temperature range of the SCGCDW phase. This suggests the existence of the domain structure in which the CDW is almost commensurate.

4. The Kohn anomaly phonon energy above the CDW transition temperature was obtained from the lower energy foot of the second order Raman peak.

References