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X-Ray TDS Study on Soft Phonon Modes of 1*T*-TaS_2

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Introduction

Charge-density-wave (CDW) formation is considered as the consequence of the electron-phonon interaction. The layered transition-metal dichalcogenides such as TaS_2 have attracted much interest because of their unique electron properties associated with quasi-two-dimensional characters and phase transitions related to the CDW formation. 1*T*-TaS_2 has three stable phases, which are an incommensurate phase (IC), a nearly commensurate phase (NC) and a commensurate phase (C) with phase-transition temperatures of 350 K (IC to NC) and 190 K (NC to C) [1,2].

Synchrotron x-ray thermal diffuse scattering (TDS) relates to the dispersion curves of phonons and quantitatively to the frequency and wavelength of traveling elastic waves in a crystal. Since the thermal vibration of the lattice can be described by a linear superposition of these waves, the TDS intensity gives the phonon dispersion curves [3].

Experimental

The TDS intensity of the IC phase was measured at the BL-10A station of Photon Factory. Single crystals of 1*T*-TaS_2 were synthesized by the chemical vapor-transport method [4]. A single crystal in dimensions of 5 x 5 x 0.2 mm^3 was mounted with a small furnace in a vertical-type four-circle diffractometer.

A satellite reflection was observed at $\boldsymbol{q} = 0.28\boldsymbol{a}^* + \boldsymbol{c}^*/3$. The TDS intensity around the 1 -1 0 reciprocal lattice point was measured within the temperature range between 300 and 460 K.

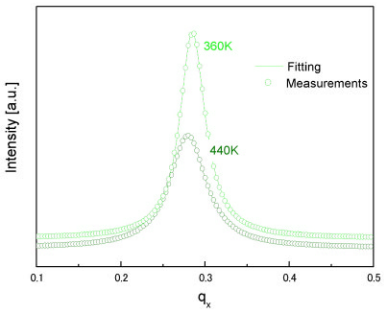

Fig. 1: TDS intensity along Γ'-M' direction. Solid lines are fitting results.

Results and discussion

Figure 1 shows the observed TDS intensities along Γ'-M' direction at 440 and 360 K, where the Bragg scattering intensities are subtracted. We applied a force constant model explain the observed TDS intensity, based on the lattice dynamics by Born and von Karman.

By using the optimized force constants, the longitudinal acoustic (LA) and transverse acoustic ($TA_{//}$) modes are calculated in the wide region including the symmetry points Γ', M' and K' in the first Brillouin zone. The LA mode is deeply softened around $q_x = 0.28$. In contrast, the $TA_{//}$ mode is softened on the circular region with the radius of 0.28. The calculated intensity distribution well reproduces the feature of the experimental data (Fig. 2). The peak at $q_x = 0.28$ can be defined as the softened LA modes to be main driving phonon for the IC-CDW. The circularly distributed diffuse streaks are associated with the softened $TA_{//}$ modes.

Thus, least-squares analyses in terms of lattice dynamics yielded the dispersion curves of phonons, which revealed the Kohn anomaly both in LA and $TA_{//}$ modes. The softened LA mode modulates the parent 1*T* structure to the IC phase. The softened $TA_{//}$ mode induces the rotation of ordering vector related to the IC to NC phase transition.

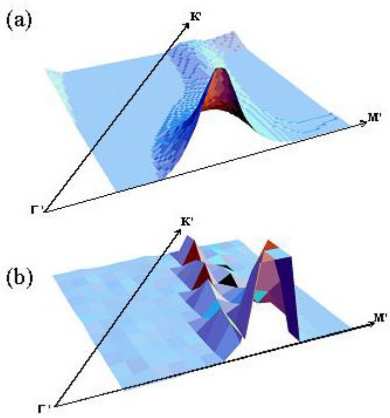

Fig. 2: TDS in G'-K'-M' section. (a) Calculated and (b) Experimental result of intensity distribution at 360 K.

References

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