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Lattice Dynamics of 1T-$TaTe_2$

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ABSTRACT

The charge density wave system 1T-$TaTe_2$ is a current topic of interest due to its interesting phase change phenomenon at the transition temperature. In this study, the theoretically calculated values of specific heat capacity, thermal conductivity and Debye Waller factor of 1T-$TaTe_2$ in both the normal and CDW phases have been reported. Present results account the phase change phenomenon in agreement with the experimental results.

Key words: Phase change phenomenon, specific heat, debye waller factor, thermal conductivity

INTRODUCTION

Charge Density Wave (CDW) phenomena have been observed predominantly in transition metal dichalcogenide layered compounds (Rossnagel, 2011; Zhu *et al*., 2015). The electron-phonon coupling (Gor'kov, 2012; Sadowski *et al*., 2013; Zhu *et al*., 2015) triggers the phase transition in these compounds, because of lattice instability and in-turn results in abnormal variation in their thermal properties. One of the 1T phase layer structured transition metal dichalcogenides namely 1T-$TaTe_2$ exhibits charge density wave phenomena below 180 K. This compound has similar crystal structure like CdI_2 with octahedral coordination between the transition metal ion and six chalcogen atoms (Wilson *et al*., 1974). Van der walls type of interaction exists between the three layers of this compound. A Commensurate Charge Density Wave (CCDW) super lattice of size $3\sqrt{3}a_0 \times a_0 \times c_0$ has been observed below 180 K for this compound (Sharma *et al*., 2002).

Phonon dispersion curves for the normal phases of 1T-TaS_2 compound were calculated by Takaoka and Motizuki (1980) using rigid ion model and shell model which is applicable for this compound also. The phonon dispersion curves and specific heat capacity variation with temperature have been calculated for the normal and CDW phases employing Born-Von Karmann formalism with necessary boundary conditions.

Neutron Scattering experiments have been performed by Di Salvo *et al*. (1976) in which they observed the new phonon modes in the first Brillouin zone as an effect of charge density wave induced atomic displacements.

From literature, it is clear that this system is a subject of much experimental study than theoretical study. Hence in this work; the theoretically calculated values of Debye Waller factor B(k) for various temperatures for both types of atoms in both phases have been reported. In addition to this the worked out thermal conductivity values for various temperatures in both phases have also been presented.

MATERIALS AND METHODS

Method of calculation: Based on the Born von Karman formalism, the dynamical matrix was constructed using the force constants evaluated by employing Pawley's potential

(Dietrich *et al*., 1975) and optic phonons. The calculated force constant values in units of 10^4 dynes cm^{-1} has presented below:

$$A = -2.0415,\ E = -2.6164,\ B_2 = -0.2045$$
$$A_2 = 0.3917,\ C = 0.4417,\ D = -0.1712$$

The diagonalization of dynamical matrix of the order (18×18) yields the eigenvalues and the eigenvectors. Using the calculated phonon frequency modes, the normal phase properties were computed for 84 wave vector points derived from the Brillouin zone Di Salvo *et al*. (1976). For the CCDW phase the computation is done for a set of 180 wave vector points obtained using folding technique. With the computed phonon frequency distribution, all the three thermal properties of 1T-$TaTe_2$ have been computed.

RESULTS AND DISCUSSION

The distribution of computed frequency modes are depicted in Fig. 1. The * and • marked curves respectively are for the normal and CCDW phases. It can be noted from the frequency distribution curves that the peaks in the CCDW phase have shifted slightly from that of normal phase. There are no reported values of phonon frequency distribution for this system available in the literature. Hence, this study's result is compared with the curves for 1T-$TiSe_2$ and 1T-TaS_2, which is of the same structure. In the case of 1T-$TiSe_2$ the phonon frequency modes were concentrated in the higher frequency modes comparing to normal phase. Similarly, in 1T-$TaSe_2$ more number of frequencies is distributed in the higher frequency domain in CCDW phase in comparison with regular phase (Balaguru *et al*., 2001). Presented results from this study also behaved in the same way.

The specific heat capacity values for different temperatures have been calculated for both the phases using the phonon frequencies of these phases. The specific heat capacity versus temperatures curve is shown in Fig. 2. The curve shows a normal behaviour except a discontinuity at the transition temperature 180 K. Hence, this curve supports the phase change phenomenon (Balaguru *et al*., 2002).

Using these phonon, frequencies and eigen vectors the Debye Waller factors for Ta and Te atoms for both phases were calculated is depicted in Fig. 3. The mark ⊕ is for Ta atom and the * mark is for Te atom. An abnormal transition was observed at the phase transition temperature. At the phase transition, for Ta atoms there is a slight decrease in W (k) but for the Te atoms there

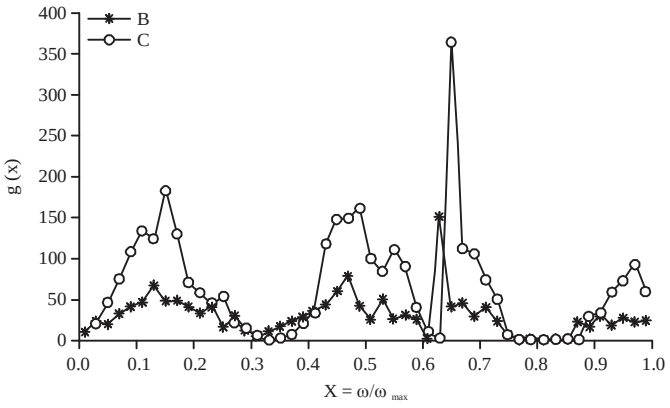

Fig. 1: X versus g(x) frequency distribution curves

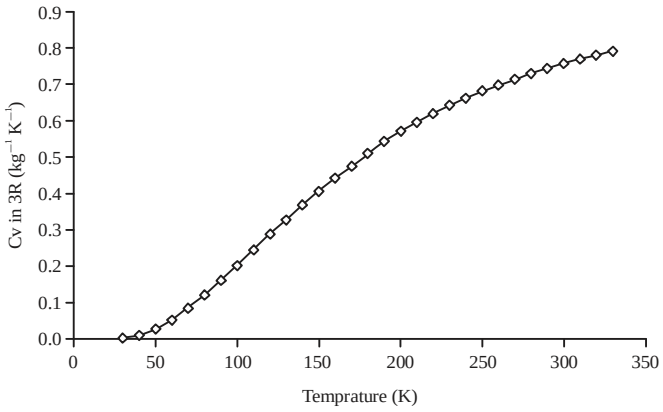

Fig. 2: Specific heat capacity versus temperature

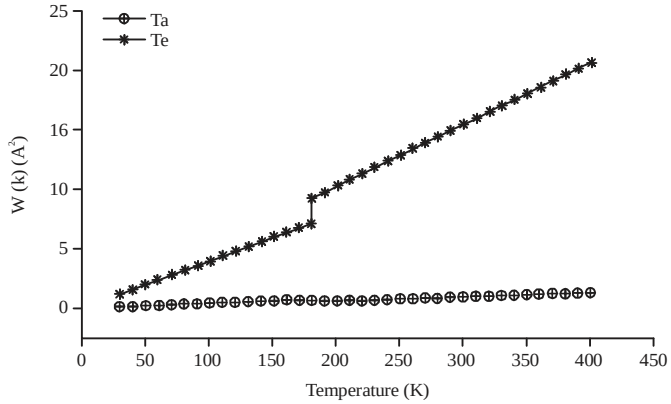

Fig. 3: Debye-Waller factor for Ta(⊕) and Te(*)

is an increase of this factor. But an interesting abnormal behaviour has been observed in CCDW phase. Based on this phase higher mass Te has high value and lower mass Ta has low value is reported. This may be attributed to the change in peak position in the frequency distribution curve in CCDW phase.

The estimated thermal conductivity values of 1T-$TaTe_2$ are graphed in Fig. 4. This curve also shows an interesting discontinuity at the transition temperature. Moreover, the thermal conductivity values have been found to be high in the low temperature region. This might be the result of increased number frequency modes in the CCDW phase.

There are neither experimental nor other theoretical results available to compare this work results with them. A similar result has been found for 1T-TaS_2 (Rayappan *et al*., 2010).

This study has been compared the onset of CDW in the 1T type transition metal dichalcogenides like 1T-TaS_2 (Takaoka and Motizuki, 1980; Rayappan *et al*., 2010), 1T-$TaSe_2$ (Balaguru *et al*., 2001), 1T-$TiSe_2$ (Di Salvo *et al*., 1976; Takaoka and Motizuki, 1980). The variations in the transition temperature play a significant role in determining the CDW induced phase transitions. In addition, the structure variations of supper lattice (Di Salvo *et al*., 1976) decide the number modes of vibrations in-turn decide the thermal properties like specific heat capacity, thermal conductivity, etc. of these layered compounds.

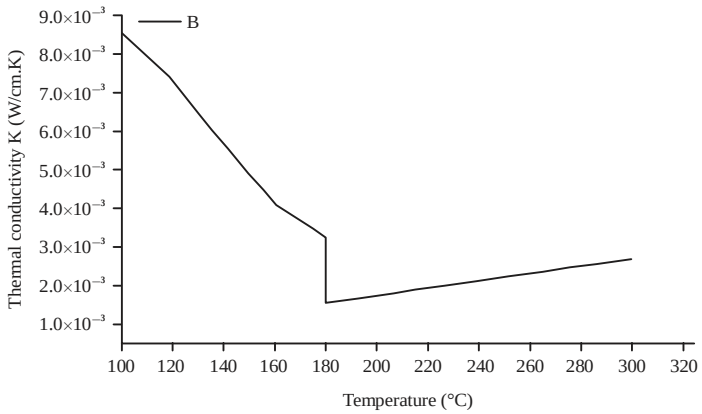

Fig. 4: 1T-$TaTe_2$ thermal conductivity results

CONCLUSION

The phonon frequency distribution of the charge density wave system 1T-$TaTe_2$ was computed for a set 84 wave vector points. The computed frequency distributions of both the phases were used to compute the thermal properties of 1T-$TaTe_2$. The computed results were compared with the existing results.

REFERENCES

Balaguru, J.B., N. Lawrence and S.A.C. Raj, 2001. Specific study on 1T-$TaSe_2$ in the context of commensurate charge density wave. Phys. Status Solidi, 223: 779-784.

Balaguru, R.J.B., N. Lawrence and S.A.C. Raj, 2002. Lattice Instability of 2H-$TaSe_2$. Int. J. Mod. Phys. B, 16: 4111-4125.

Di Salvo, F.J., D.E. Moncton and J.V. Waszczak, 1976. Electronic properties and superlattice formation in the semimetal $TiSe_2$. Phys. Rev. B, 14: 4321-4328.

Dietrich, O.W., G.A. Mackenzie and G.S. Pawley, 1975. The structural phase transition in solid DCN. J. Phys. C: Solid State Phys., 8: L98-L102.

Gor'kov, L.P., 2012. Strong electron-lattice coupling as the mechanism behind charge density wave transformations in transition-metal dichalcogenides. Phys. Rev. B, Vol. 85.

Rayappan, J.B.B., S.A.C. Raj and N. Lawrence, 2010. Thermal properties of 1T-TaS_2 at the onset of charge density wave states. Phys. B: Condensed Matter, 405: 3172-3175.

Rossnagel, K., 2011. On the origin of charge-density waves in select layered transition-metal dichalcogenides. J. Phys.: Condensed Matter, Vol. 23. 10.1088/0953-8984/23/21/213001

Sadowski, J.W., K. Tanaka and Y. Nagai, 2013. Effects of band structure and electron-phonon coupling on charge density waves. Can. J. Phys., 91: 487-489.

Sharma, S., L. Nordstrom and B. Johansson, 2002. Stabilization of charge-density waves in 1T-TaX_2(X=S,Se,Te): First-principles total energy calculations. Phys. Rev. B, Vol. 66. 10.1103/PhysRevB.66.195101

Takaoka, Y. and K. Motizuki, 1980. Lattice Dynamics of 1*T*-$TiSe_2$. J. Phys. Soc. Jpn., 49: 1838-1844.

Wilson, J.A., F.J. di Salvo and S. Mahajan, 1974. Charge-density waves in metallic, layered, transition-metal dichalcogenides. Phys. Rev. Lett., 32: 882-885.

Zhu, X., Y. Cao, J. Zhang, E.W. Plummer and J. Guo, 2015. Classification of charge density waves based on their nature. Proc. Natl. Acad. Sci., 112: 2367-2371.