# Engineering of Charge Density Wave behavior in $NdTe_3$

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## Abstract

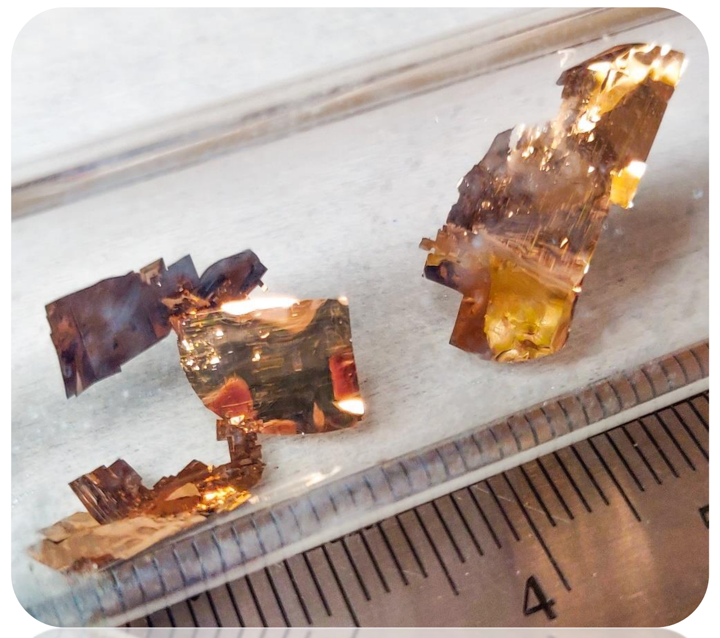
In the Lanthanum based Tri-telluride family, $RTe_3$s [R=La, Ce, Nd, Sm, Gd, Tb, Dy, Er, Ho, Tm] the emergence of Charge Density Waves (CDWs) has been under investigation for a long time due to anisotropy of the crystal and incompletely filled 4f-orbital. Confirming the CDW states in $RTe_3$s and understanding their behavior as a function of variable parameters, like temperature, will help in speculating the performance of $RTe_3$ as a superconductor. Elemental Neodymium and Tellurium, along with Iodine as transport agent will be used in synthesis by Chemical Vapor Transport, which will result in single crystals of $RTe_3$. Then These $RTe_3$s were characterized to confirm CDW states by the presence of Phonon Softening and CDW transition temperature by couple-model.

## Background

Typically, in metals, the equilibrium position of ions forms a perfectly periodic lattice, and the electron density is highly uniform. When the temperature is changed, the Fermi Surface (FS) of some metals becomes unstable above/below a certain transition temperature (Tc); this instability results in redistribution of charge density thereby forming periodic space modulation. Such a periodic space modulation is termed as Charge Density Waves (CDW). This modulation of charge density alters the ion potential in the lattice leading to the movement of ions to a new equilibrium position, as a result, a CDW is accompanied by periodic lattice distortion. The phonon mode attained by the wave vector around $q=2K_f$ will be renormalized to vibrate at lower energy on account of divergence of response at that wave vector. This kind of phonon renormalization is called phonon softening.

## Materials and synthesis method

Single crystals of $NdTe_3$ are successfully grown with CVT, for the first time, with elemental (99.9%purity by Alfa Aesar) Neodymium, Tellurium and Iodine as Transport agent. All the precursors were filled in a quartz ampoule; the ampoule was vacuum sealed and then the ampoule was kept in a two-zone furnace at an effective temperature of 832℃ at source and 690℃ at sink for 96 hours. Refer to Fig. 1 for crystal size.



## Results, Discussions and Conclusion

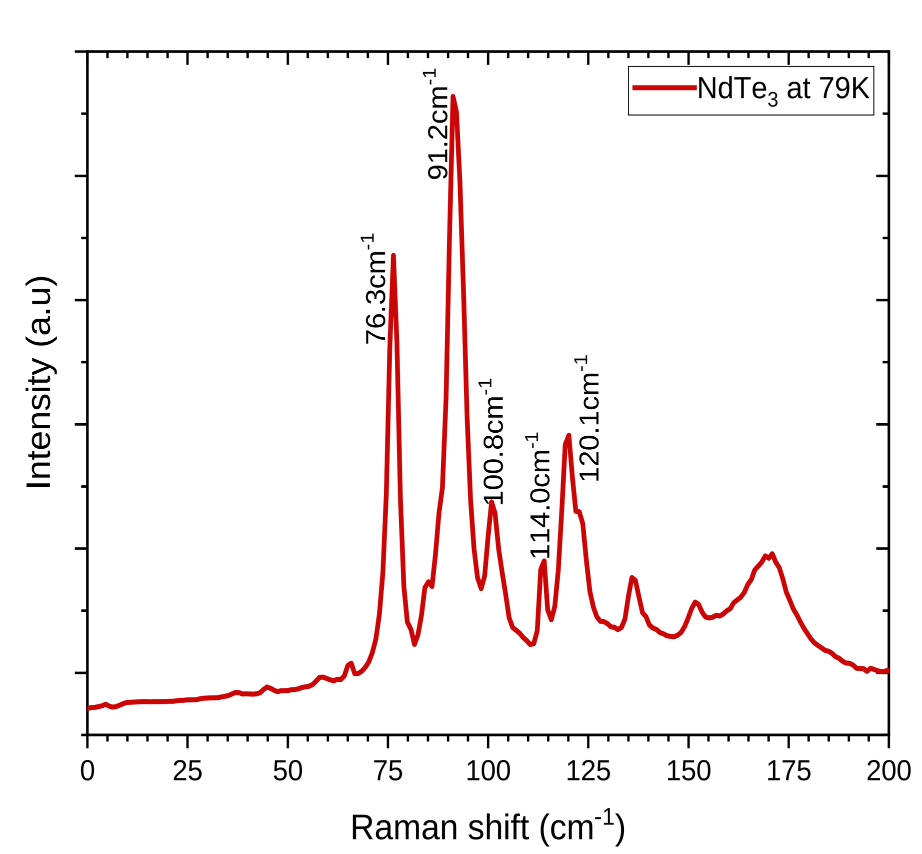



Fig. 2: Raman spectroscopy of $NdTe_3$ at 79K

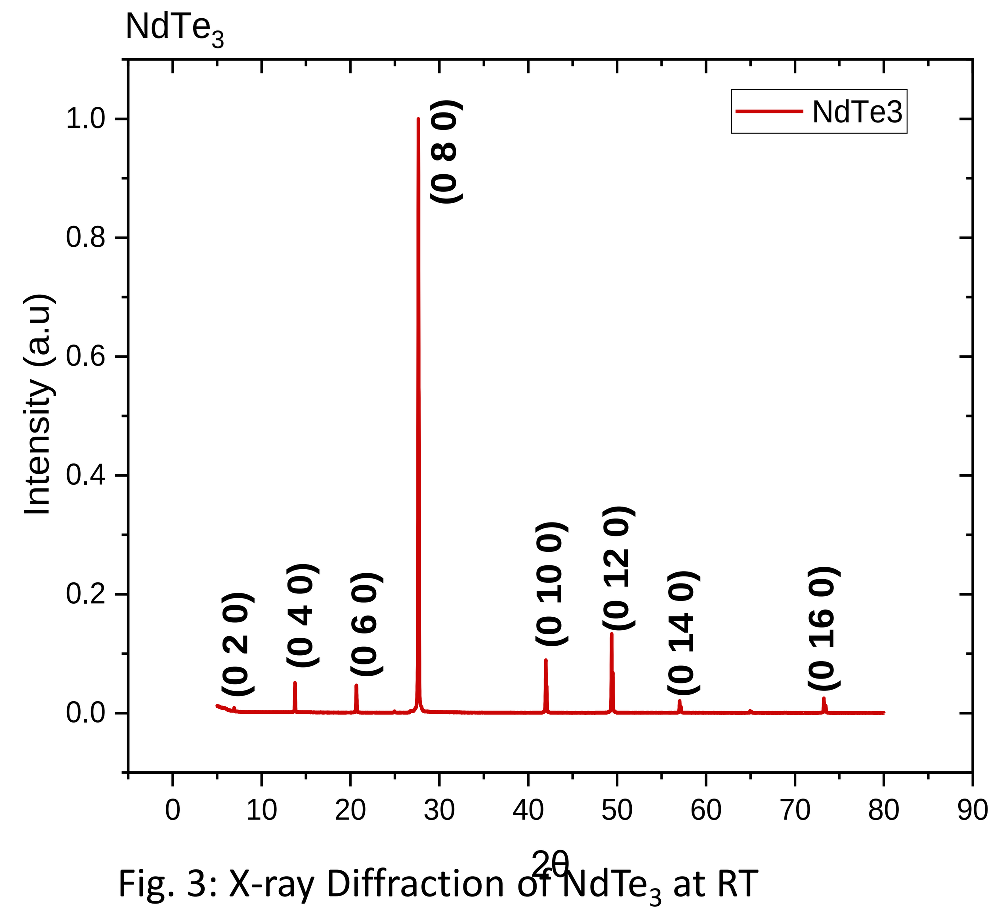



Fig. 3: X-ray Diffraction of $NdTe_3$ at RT

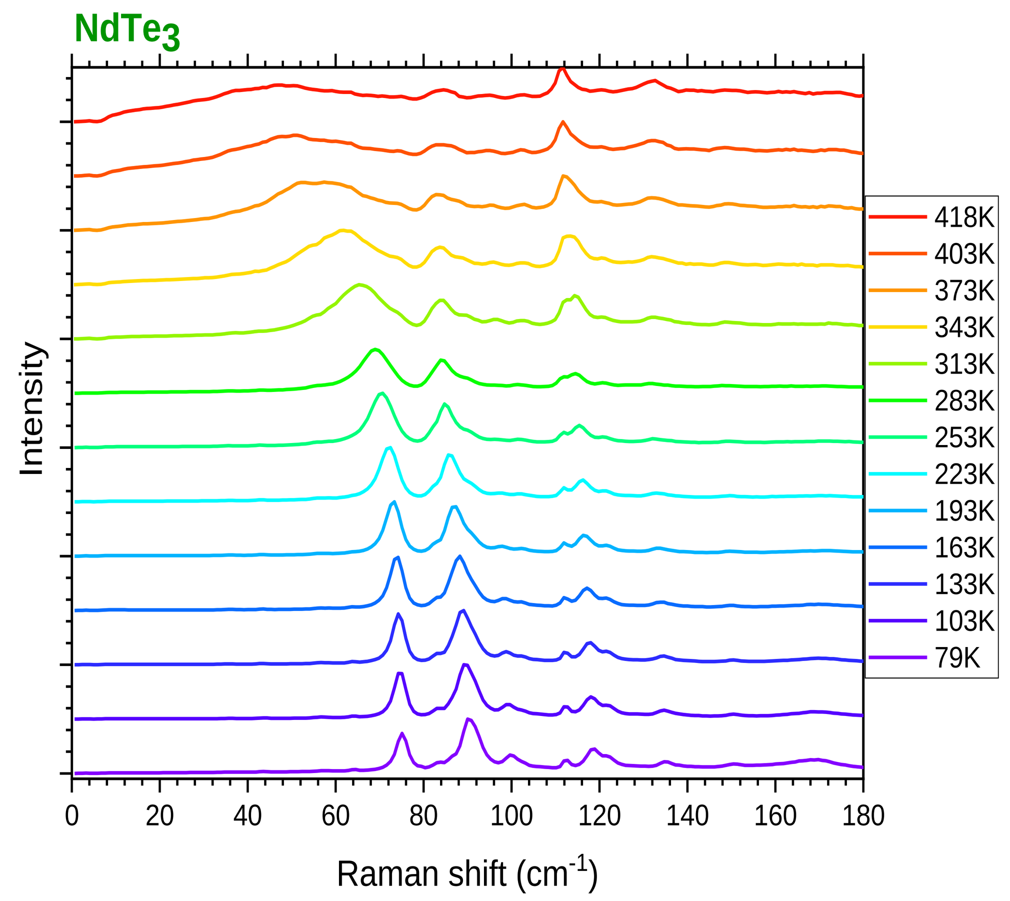



Fig. 3: Temperature dependent Raman spectroscopy of $NdTe_3$

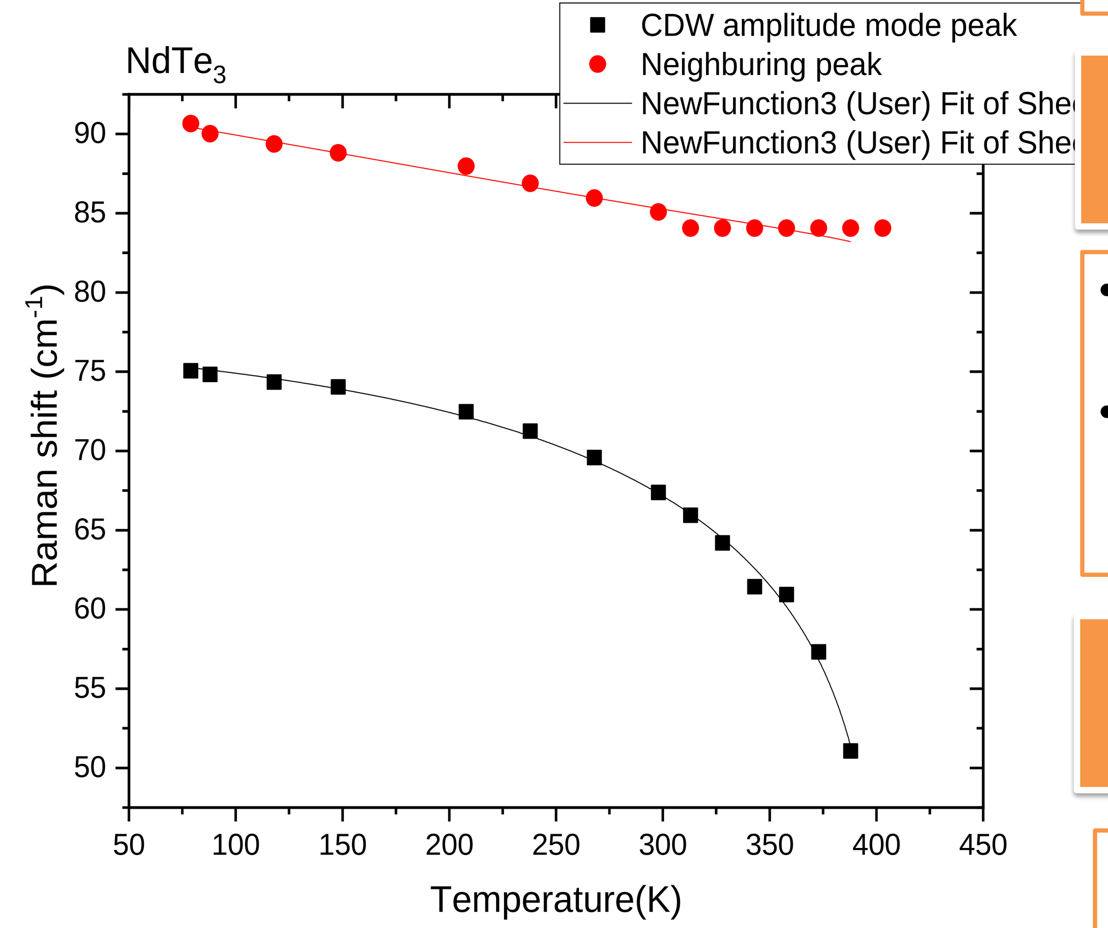



Fig 4: CDW calculation by coupling model

- Fig. 2 showing the Raman Spectra of the grown crystal; Fig. 3 showing the diffracted peaks from XRD confirms the crystal is $NdTe_3$ with (0 1 0) orientation from literature.
- Fig. 4 shows temperature dependent Raman spectrum from 79K to 418K; the peak at 76.3 and 91.2 $cm^{-1}$ are the CDW amplitude mode peak and neighboring peak. As temperature increases, the peaks move towards lower frequencies/energies. The temperature at which the CDW peak shifts to zero frequency is known as CDW transition temperature.
- Fig. 5 shows the fitting of CDW peak position as a function of temperature, thereby resulting in temperature where CDW peak is at zero frequency i.e $T_{cdw}$= 403K.

## Conclusion

- $NdTe_3$ crystal was successfully grown by CVT, as confirmed from Raman Spectroscopy and XRD.
- Temperature dependent Raman spectroscopy shows phonon-softening and was used to calculate CDW transition temperature by couple model.

## Future work

- Functionalization of $NdTe_3$ to prevent environmental degradation
- Magnetic measurement to find magnetic ordering for physical property identification.
- R vs T measurement to find out $T_{cdw}$ by electrical field; this study couple with phonon softening could provide with a comparative study of CDW attained by heat and electric field.
- Thickness dependence of $T_{cdw}$, by monolayer exfoliation of $NdTe_3$ .

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## References

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