

Abstract

Ferromagnetic and ferroelectric materials undergo phase transitions that allow them to maintain remnant magnetization or electrical polarization at low temperatures, even in the absence of an external field. It has been observed that the introduction of defects in the crystal lattice promotes the appearance of ferroic orders. Recently, a multiferroic transition at room temperature was observed in Te-doped transition metal dichalcogenide WSe_2 , where the material exhibited the coexistence of ferroelectric and ferromagnetic orders, with a significant influence of vacancies on the emergence of these properties. Based on these studies, it is proposed that similar materials, such as $Mo(Se_{1-x}Te_x)_{2(1-\delta)}$, could exhibit analogous behaviors.[1, 2]

1. Introduction

Recently, room temperature multiferroicity was observed on the solid solution $W(Se_{1-x}Te_x)_{2(1-\delta)}$ where x represents the Te doping and δ the chalcogen vacancies, this composite was formed by the combination of the semimetal WSe_2 and the semiconductor WTe_2 [3]. The analysis of multiple stoichiometric variations for this solution showed that the doping promoted the formation of vacancies, which showed to be crucial for the presence of ferroic orders.

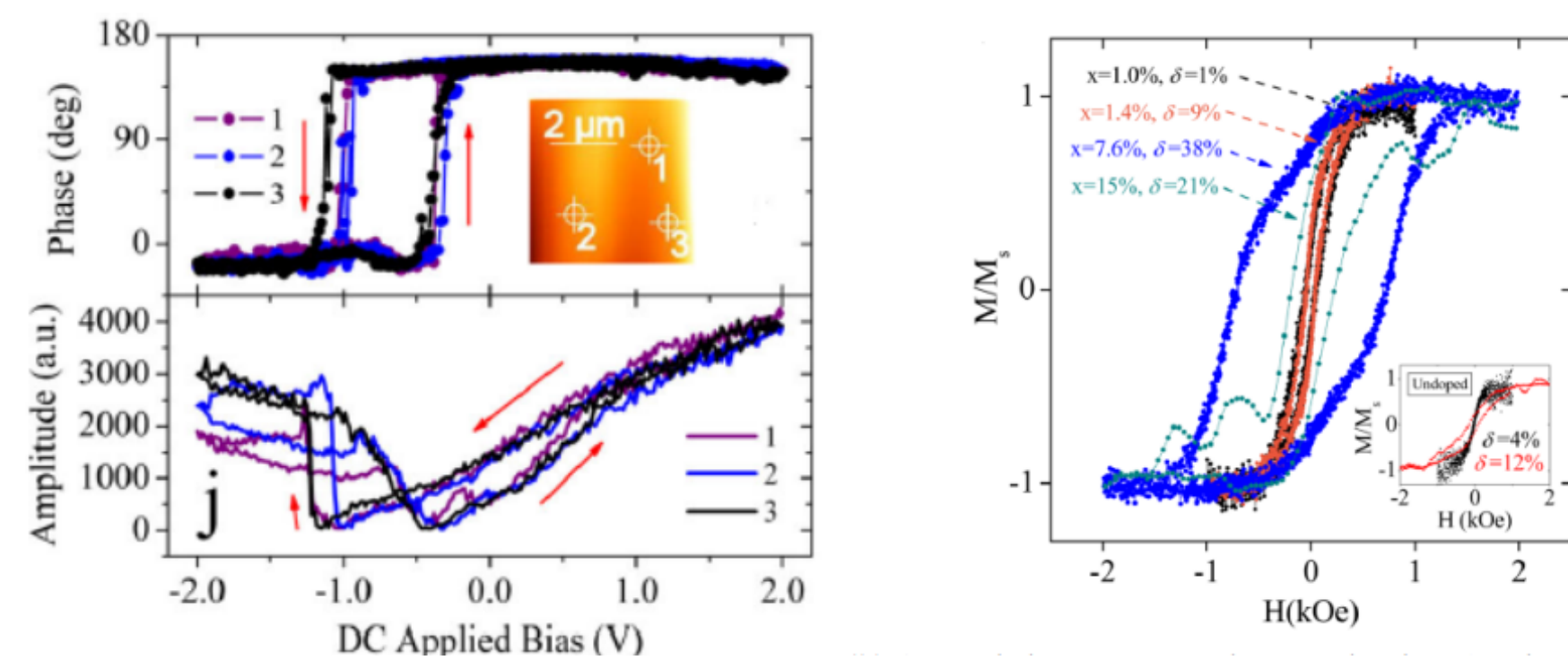


Fig. 1: PFM and VSM curves for different compositions of $W(Se_{1-x}Te_x)_{2(1-\delta)}$, both curves show the hysteresis characteristic of ferroic orders.

2. Experimental Methods

1. Crystal growth:

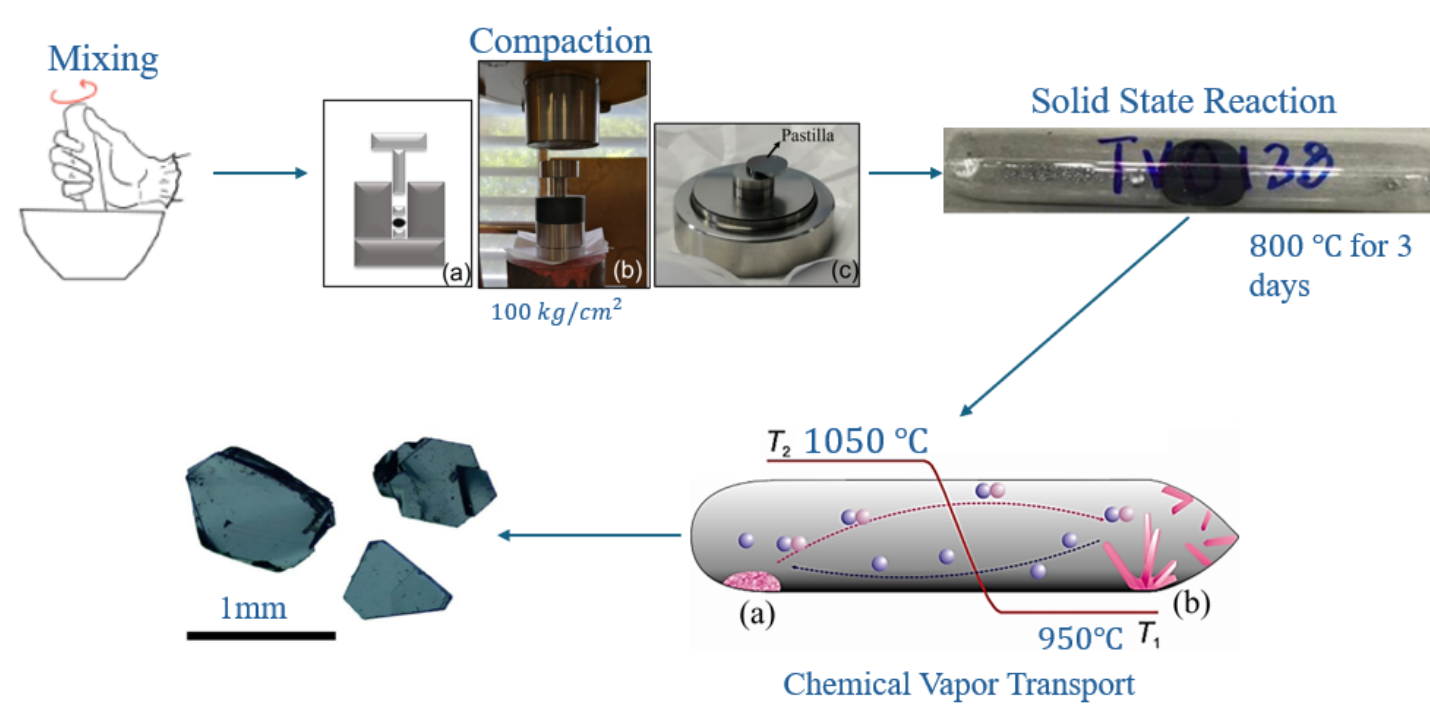


Fig. 2: Main stages of the growth process for the $Mo(Se_{1-x}Te_x)_{2(1-\delta)}$ crystals.

2. Techniques used for characterization:

- X-Ray Diffraction (XRD) and Raman spectroscopy: To observe changes in the crystal structure due to the introduction of defects.
- X-Ray fluorescence: To determine the stoichiometry of different samples.
- Vibrating sample magnetometry and piezoelectric force microscopy: To analyze the magnetic and electric orders in different solutions.

3. Results

XRD results for multiple compositions of $Mo(Se_{1-x}Te_x)_{2(1-\delta)}$ show that the main diffraction peaks correspond to the (00l) family of planes, which display a shift in the 2θ angle where the peaks are located. Since these planes are directly related to the lattice parameter c , the shift represents a variation in the magnitude of c . In the second figure, it can be observed that the lattice parameter c increases with the amount of doping in the samples.

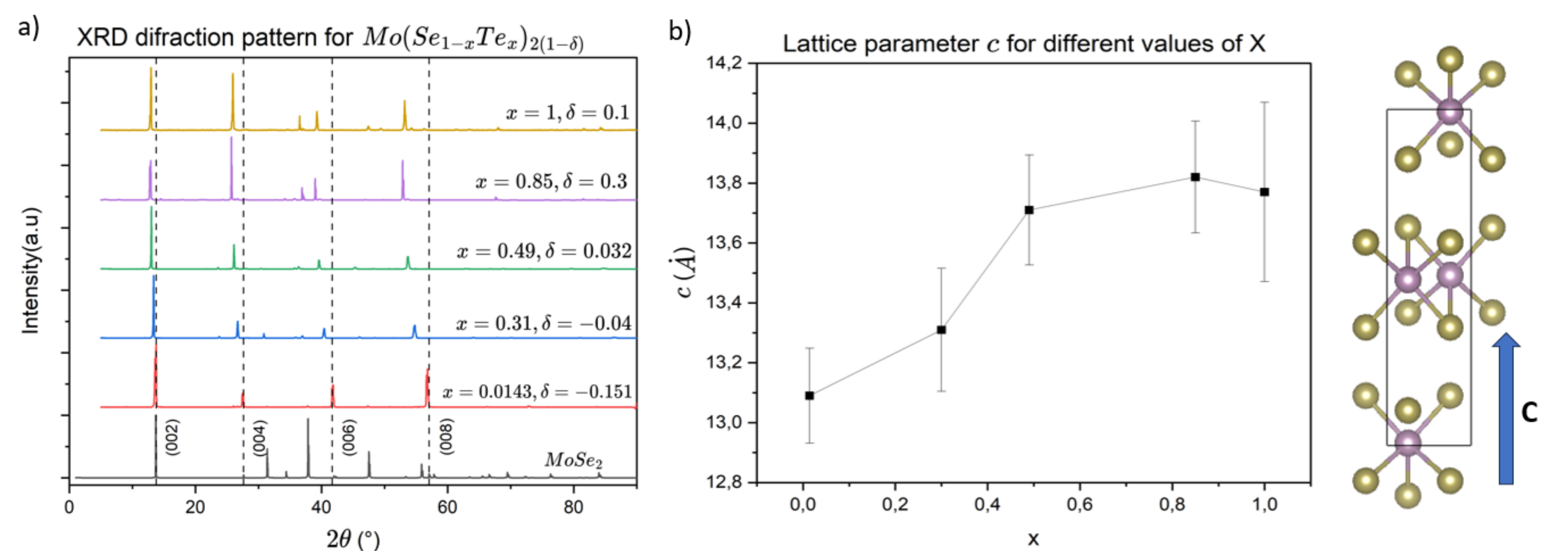


Fig. 3: a) shows the XRD pattern for multiple solutions of $Mo(Se_{1-x}Te_x)_{2(1-\delta)}$ compared to the expected peaks for $MoSe_2$. b) shows the calculated values for the lattice parameter c , based on the observed diffraction pattern.

The Raman spectra for multiple compositions of $Mo(Se_{1-x}Te_x)_{2(1-\delta)}$ show that the dominant phase in the solutions varies depending on the doping level. It was observed that this dominant phase corresponds to the pure composition closest to the one under analysis. Furthermore, for compositions closer to $MoTe_2$, peaks associated with both the 2H and 1T' crystal phases were observed, indicating a coexistence of crystal phases, with the 1T' phase being dominant.

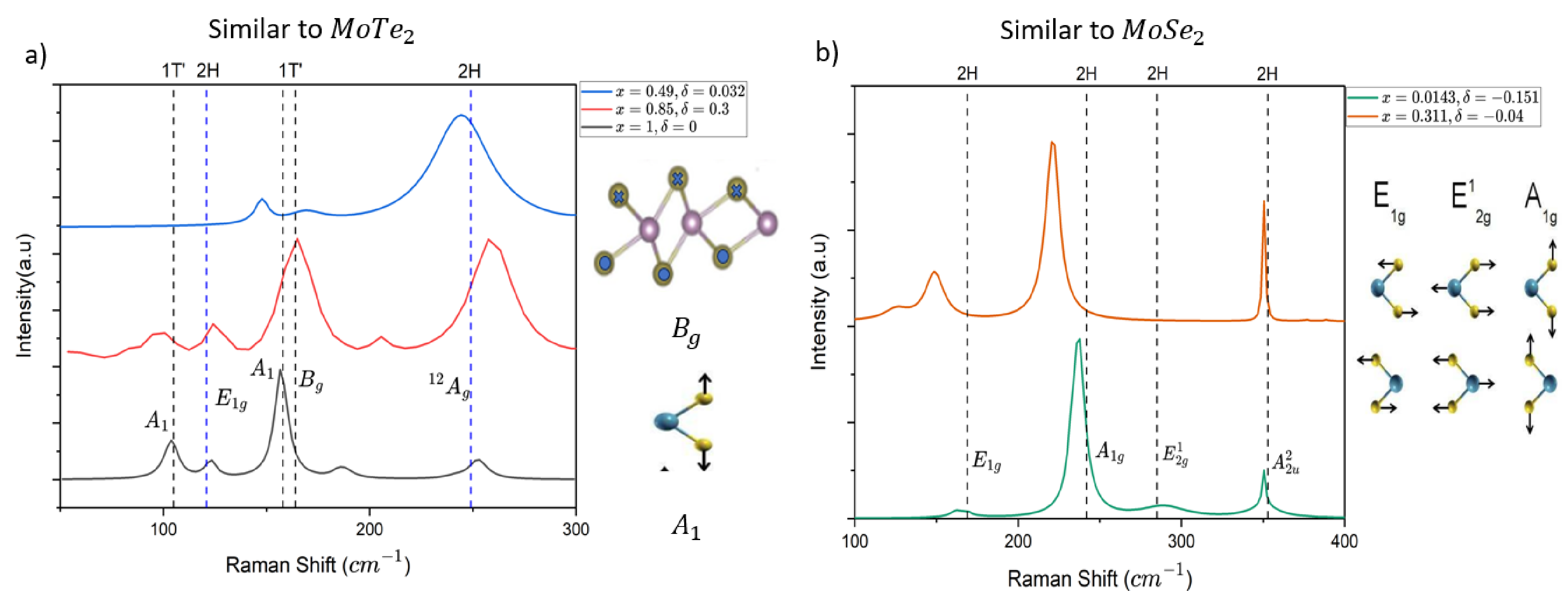


Fig. 4: The Raman spectra for multiple compositions of $Mo(Se_{1-x}Te_x)_{2(1-\delta)}$ show that the dominant phase in the solutions changes with the doping level. Figure (a) presents the Raman spectrum that most closely resembles that of pure $MoTe_2$ compared to the expected peaks (vertical lines), along with a representation of the B_g and A_1 Raman modes. It can be observed that some peaks correspond to different crystal phases. Figure (b) presents the Raman spectrum that most closely resembles $MoSe_2$ in its 2H crystal phase compared to the expected peaks (vertical lines), along with a representation of the A_{1g} and E_g Raman modes.

Both sets of results indicate that the introduction of crystal defects significantly alters the crystal structure, changing the dominant crystal phase. This causes effects such as an increase in lattice parameters and the breaking of centrosymmetry due to the transition to the 1T' phase.

4. Conclusions and future work

The crystallographic analysis shows that doping effectively distorts the crystal structure, altering both the lattice parameters and the crystal phase, indicating a breaking of centrosymmetry in the system. This symmetry breaking is identified as a factor inducing spontaneous polarization in crystal systems. Future work should focus on identifying the direct effect of vacancies on the crystal structure by producing compositions with more controlled vacancies. In parallel with crystal structure analysis, the effects of both doping and vacancies on the ferroic orders of the solution remain to be analyzed.

References

- [1] Yuan, S. *et al.* Room-temperature ferroelectricity in $MoTe_2$ down to the atomic monolayer limit. *Nature Communications* **10** (2019).
- [2] Xia, B. *et al.* Phase-transfer induced room temperature ferromagnetic behavior in 1T@2H- $MoSe_2$ nanosheets. *Scientific Reports* **7** (2017).
- [3] Cardenas-Chirivi, G. *et al.* Room temperature multiferroicity in a transition metal dichalcogenide. *npj 2D Materials and Applications* **7**(54) (2023).