Synthesis and Characterization of Polycrystalline $NbTe_2$: Exploring Phase Formation and Stability

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Abstract

Transition-metal dichalcogenide, $NbTe_2$, as a quantum material has attracted a lot of attention due to its promising electronic and optical properties and potential applications. Despite extensive studies on $NbTe_2$, synthesis of high-quality, single-phase polycrystalline $NbTe_2$ remains a challenge. Polycrystalline materials offer distinct advantages over single crystals, including ease of synthesis, scalability, and excellent mechanical properties. Here we are addressing the limitations of single-crystal dominated research, such as lack of detailed powder diffraction analysis and absence of precise boundaries of two-phase regions between different phases of polycrystalline $NbTe_2$, crucial to optimizing synthesis conditions and achieving phase purity. We investigated the phase stability of polycrystalline $NbTe_2$ through controlled synthesis by varying reaction time from 72 hrs to 120 hrs and modifying temperature profiles ranging from 550c to 700c. The Rietveld refinement of *x*-ray diffraction data reveals that pure phase polycrystalline $NbTe_2$ crystallises in monoclinic structure with $P2_1/m$ space group and lattice parameters a = 3.638 Å, b = 9.314 Å, c = 14.664 Å, β = 110.07 º, α = γ = 90º. Raman spectra obtained using excitation wavelength of 532 nm further corroborated phase formation. while elemental composition was confirmed via energy-dispersive *x*-ray spectroscopy. This study provides a basis for further research on polycrystalline $NbTe_2$ as a quantum material.