Materials Science and Engineering Master's Defense

Angle Resolved Polarization and Vibrational Studies of Transition Metal Trichalcogenides and Related Alloys

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abstract

A new class of layered materials called the transition metal trichalcogenides (TMTCs) exhibit strong anisotropic properties due to their quasi-1D nature. These 2D materials are composed of chain-like structures which are weakly bound to form planar sheets with highly directional properties. The vibrational properties of three materials from the TMTC family, specifically TiS_3, ZrS_3, and HfS_3, are relatively unknown and studies performed in this work elucidates the origin of their Raman characteristics. The crystals were synthesized through chemical vapor transport prior to mechanical exfoliation onto Si/SiO_2 substrates. XRD, AFM, and Raman spectroscopy were used to determine the crystallinity, thickness, and chemical signature of the exfoliated crystals. Vibrational modes and anisotropic polarization are investigated through density functional theory calculations and angle-resolved Raman spectroscopy. Particular Raman modes are explored in order to correlate select peaks to the b-axis crystalline direction. Mode III vibrations for TiS_3, ZrS_3, and HfS_3 are shared between each material and serves as a unique identifier of the crystalline orientation in MX_3 materials. Similar angle-resolved Raman studies were conducted on the novel $Nb_{0.5}Ti_{0.5}S_3$ alloy material grown through chemical vapor transport. Results show that the anisotropy direction is more difficult to determine due to the randomization of quasi-1D chains caused by defects that are common in 2D alloys. This work provides a fundamental understanding of the vibrational properties of various TMTC materials which is needed to realize applications in direction dependent polarization and linear dichroism.

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