

THEORETICAL AND CONDENSED MATTER PHYSICS

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Structural and optical properties of the MoTe₂-WTe₂ alloy system

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The structural polymorphism intrinsic to transition metal dichalcogenides provides exciting opportunities for engineering novel devices. Of special interest are memory technologies that rely upon controlled changes in crystal phase, collectively known as phase change memories (PCMs). MoTe₂ is ideal for PCMs as the ground state energy difference between the hexagonal (2H, semiconducting) and monoclinic (1T', metallic) phases is minimal. This energy difference can be further reduced by substituting W for Mo on the metal sublattice, thus improving PCM performance. Therefore, understanding the properties of Mo_{1-x}W_xTe₂ alloys across the entire compositional range is vital for the technological application of these versatile materials. We combine Raman spectroscopy with aberration-corrected scanning transmission electron microscopy and x-ray diffraction to explore the MoTe₂-WTe₂ alloy system. The results of these studies enable the construction of the complete alloy phase diagram, while polarization-resolved Raman measurements provide phonon mode and symmetry assignments for all compositions. Temperature-dependent Raman measurements indicate a transition from 1T'-MoTe₂ to a distorted orthorhombic phase (T_d) below 250 K and facilitate identification of the harmonic contributions to the optical phonon modes in bulk MoTe₂ and Mo_{1-x}W_xTe₂ alloys. We also identify a Raman-forbidden MoTe₂ mode that is activated by compositional disorder and find that the main WTe₂ Raman peak is asymmetric for x < 1. This asymmetry is well-fit by a phonon confinement model, which allows the determination of the phonon correlation length. Our work is foundational for future studies of Mo_xW_{1-x}Te₂ alloys and provides new insights into the impact of disorders in transition metal dichalcogenides.

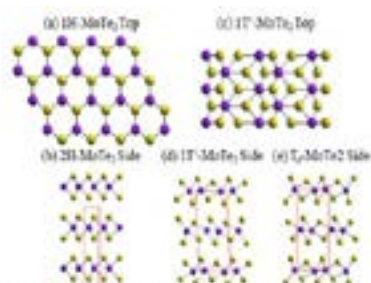


Figure 1: (a) Top and (b) side views of MoTe₂ in the 1H (monolayer) and 2H (bulk) structural phase. (c) top view of monolayer 1T' MoTe₂. (d,e) side view of bulk MoTe₂ in the 1T' and T_d structural phase.

Biography

Patrick M Vora has received a PhD in Physics from the University of Pennsylvania. Subsequently, he was a Postdoctoral Fellow at the University of Pennsylvania and later at the US Naval Research Laboratory as a part of the National Research Council's Research Associateship Program. He was named an Assistant Professor at George Mason University in 2014 where he has established a research group that focuses on two-dimensional materials. He has published 22 papers in reputed journals.

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