Materials Science & Engineering Doctoral Defense

Novel Growth Routes and Fundamental Understanding of Pseudo-One-Dimensional Materials

School for Engineering of Matter, Transport and Energy

Kedi Wu

Advisor: Sefaattin Tongay

abstract

Recently, two-dimensional (2D) materials have emerged as a new class of materials with highly attractive electronic, optical, magnetic, and thermal properties. However, there exists a sub-category of 2D layers wherein constituent metal atoms are arranged in a way that they form weakly coupled chains confined in the 2D landscape. These weakly coupled chains extend along particular lattice directions and host highly attractive properties including high thermal conduction pathways, high-mobility carriers, and polarized excitons. In a sense, these materials offer a bridge between traditional one-dimensional (1D) materials (nanowires and nanotubes) and 2D layered systems. Therefore, they are often referred as pseudo-1D materials, and are anticipated to impact photonics and optoelectronics fields. This dissertation focuses on the novel growth routes and fundamental investigation of the physical properties of pseudo-1D materials. Example systems are based on transition metal chalcogenide such as rhenium disulfide (ReS2), titanium trisulfide (TiS3), tantalum trisulfide (TaS3), and titanium-niobium trisulfide (Nb(1-x)TixS3) ternary alloys. Advanced growth, spectroscopy, and microscopy techniques with density functional theory (DFT) calculations have offered the opportunity to understand the properties of these materials both experimentally and theoretically. The first controllable growth of ReS2 flakes with well-defined domain architectures has been established by a state-of-art chemical vapor deposition (CVD) method. High-resolution electron microscopy has offered the very first investigation into the structural pseudo-1D nature of these materials at an atomic level such as the chain-like features, grain boundaries, and local defects. Pressure-dependent Raman spectroscopy and DFT calculations have investigated the origin of the Raman vibrational modes in TiS3 and TaS3, and discovered the unusual pressure response and its effect on Raman anisotropy. Interestingly, the structural and vibrational anisotropy can be retained in the Nb(1-x)TixS3 alloy system with the presence of phase transition at a nominal Ti alloying limit. Results have offered valuable experimental and theoretical insights into the growth routes as well as the structural, optical, and vibrational properties of typical pseudo-1D layered systems. The overall findings hope to shield lights to the understanding of this entire class of materials and benefit the design of 2D electronics and optoelectronics.

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