Materials Science and Engineering Thesis Defense

Alloying of 2D Anisotropic Materials and Studying Their Vibrational and Optical Properties

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abstract

Alloying in semiconductors has enabled many civilian technologies in optoelectronics, photonics fields and more. While the phenomenon of alloying is well established in traditional bulk semiconductors, owing to vastly available ternary phase diagrams, the ability to alloy in 2D systems are less clear. Recently anisotropic materials such as ReS2 and TiS3 have been extensively studied due to their direct-gap semiconductor and high mobility behaviors. This work is a report on alloys of ReS2 & ReSe2 and TiS3 & TiSe3 .Alloying selenium into ReS2 in the creation of ReS(2x)Se(2-x) , tunes the band gap and changes its vibrational spectrum. Depositing this alloy using bottom up approach has resulted in the loss of crystallinity. This loss of crystallinity was evidenced by grain boundaries and point defect shown by TEM images.Also, in the creation of TiS(3x)Se(3-x) , by alloying Se into TiS3 , a fixed ratio of 8% selenium deposit into TiS3 host matrix is observed. This is despite the vastly differing precursor amounts and growth temperatures, as evinced by detailed TEM, EDAX, TEM diffraction,and Raman spectroscopy measurements. This unusual behavior contrasts with other well-known layered material systems such as MoSSe, WMoS2 where continuous alloying can be attained. Cluster expansion theory calculations suggest that only limited composition (x) canbe achieved. Considering the fact that TiSe3 vdW crystals have not been synthesized in the past, these alloying rejections can be attributed to energetic instability in the ternary phase diagrams estimated by calculations performed. Overall findings highlight potential means and challenges in achieving stable alloying in promising direct gap and high carrier mobility TiS3 materials.

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