Materials Science & Engineering Thesis Defense

Band gap engineering and phase transition in InSeS and InSeTe Alloys

School for Engineering of Matter, Transport and Energy

Anvesh Yarra Advisor: Sefaattin Tongay

Abstract

Many important technologies, including electronics, computing, communications, optoelectronics, and sensing, are built on semiconductors. The band gap is a crucial factor in determining the electrical and optical properties of semiconductors. Beyond graphene, newly found two-dimensional (2D) materials have semiconducting bandgaps that range from the ultraviolet in hexagonal boron nitride to the terahertz and mid-infrared in bilayer graphene and black phosphorus, visible in transition metal dichalcogenides (TMDs). These 2D materials were shown to have highly controllable bandgaps which can be controlled by alloying. Only a small number of TMDs and monochalcogenides have been alloyed, though, because alloying compromised the material's Vdw property and the stability of the host crystal lattice phase. Phase transition in 2D materials is an interesting phenomenon where work has been done only on few TMDs namely MoTe2, MoS2, TaS2 etc.

In order to change the band gaps and move them towards the UV (ultraviolet) and IR (infrared) regions, this work has developed new 2D alloys in InSe by alloying them with S and Te at 10% increasing concentrations. As the concentration of the chalcogens (S and Te) increased past a certain point, a structural phase transition in the alloys was observed. However, pinpointing the exact concentration for phase change and inducing phase change using external stimuli will be a thing of the future.

The resulting changes in the crystal structure and band gap were characterized using some basic characterization techniques like SEM, XRD, Raman and PL spectroscopy.

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