The effects of doping and alloying on Molecular Beam Epitaxy-Grown Transition Metal Dichalcogenides

Popular science abstract

The discovery of graphene, an extraordinary single layer of graphite (one atom thick) with remarkable electronic and mechanical properties, has spurred extensive research on two-dimensional (2D) materials. This led to the identification of an entire family of ultra-thin materials, including semiconductors, insulators, magnetic, and topological materials. Furthermore, these materials can be stacked in van der Waals heterostructures, resembling sandwiches, to modify their electrical, optical, and magnetic properties, offering prospects for future applications and the development of microscopic devices such as transistors.

However, in the current semiconductor industry, simply combining materials to form heterostructures does not fully exploit their potential. To fine-tune the properties of semiconductors, the essential tools are doping (adding trace amounts of elements outside the parent crystal) and alloying (combining different compounds in comparable proportions). While van der Waals heterostructures can be created through mechanical exfoliation, doping and alloying heavily rely on advanced manufacturing techniques. One such technique is molecular beam epitaxy (MBE), known for its proficiency in material growth.

The objective of this project is to investigate the possibilities and consequences of doping and alloying in two-dimensional materials grown using MBE. Doping involves, for instance, replacing every hundredth molybdenum atom in $MoSe_2$ with vanadium to create a doped material called $M_{0.99}V_{0.01}Se_2$. In contrast, alloys exhibit comparable proportions of different metal atoms, such as 30% molybdenum and 70% tungsten forming the $Mo_{0.3}W_{0.7}Se_2$ alloy. Crucially, the MBE method allows for the production of a series of samples with varying compositions, enabling the observation of systematic changes associated with differences in atom concentration. We anticipate modifications in electronic structure, mechanical properties, optical responses, and magnetic characteristics.

These layered materials exhibit intriguing optical and electrical effects, particularly when studying their monolayers. Additionally, enhanced effects can be achieved by arranging these monolayers on a two-dimensional insulator like hexagonal boron nitride. The success of this project relies on the principal investigator's expertise in developing MBE growth technology for monolayers of 2D materials (e.g., $MoSe_2$, WSe_2, and (Mo, Mn)Se_2 thus far) directly on hexagonal boron nitride, resulting in structures with exceptional optical properties. This advancement will enable the observation and understanding of even the subtlest physical effects.