PROJECT SUMMARY

Overview:

Semiconductor devices are an integral part of modern life. To date, most high performance semiconductor devices are made of single-crystal films grown on single-crystal substrates. Achieving a high quality heteroepitaxial film on a single-crystal substrate requires a good lattice and/or symmetry matching between the film and substrate. Because of this restriction, only limited combinations of materials can be utilized. For covalent materials with a large lattice mismatch, the strong chemical interaction (dangling bonds) at the interface introduces defects such as dislocations to release the strain at the interface. These defects would act as recombination centers, which compromise the quality of the film's properties. In this proposal we will study the epitaxial film growth by electron diffraction and spectroscopy, in particular at the initial stages of growth by molecular beam epitaxy, of non-layered semiconductors such as CdTe on graphene substrates through weak van der Waals interactions. In contrast to the conventional chemical epitaxy in which sharing or transferring of electrons occurs at the film-substrate interface, van der Waals epitaxy (vdWE) is based on a physical Coulombic force through dipole interactions. Since there are no "dangling bonds" at the surface in vdWE junctions, it is believed that the fulfillment of the lattice matching restriction needed to grow a defect-free film in the conventional chemical epitaxy is no longer a requirement; high quality epitaxial films can be grown. This implies that the film can be incommensurate and strain can be relaxed right at the interface during growth. In addition, a recent intriguing first-principles calculations predict that if the film-substrate interaction is weak, many binary compound semiconductors such as CdTe is thermodynamically more stable in a layered structure form of double-layer honeycomb (DLHC) with novel electronic structure (similar to the single-layer honeycomb structure for graphene but double-layer) when the film is very thin, totally different from the traditional bulk zincblende structure which is a non-layered structure.

Intellectual Merit:

The question on the role of vdW interactions on the growth of traditional semiconductors such as CdTe on graphene and the possibility of a physical realization of its predicted layered structure at the ultrathin regime stimulate us to explore the use of surface sensitive techniques to explore these fundamental scientific issues such as "Is there a universal trend that all bulk materials could be synthesized as layer structure in 2D limit?" The in situ reflection high-energy electron (RHEED) technique in two modes will be employed in this study: Azimuthal RHEED in the reflection mode for smooth films supplemented by high-resolution low-energy electron diffraction, and RHEED surface pole figure technique (invented by our group) in the transmission mode for rough films. Morphology, quantitative interface strain evolution, film-graphene orientation relationship, and crystal orientation, will be determined.

Broader Impacts:

The success of the proposed work will not only allow us to gain fundamental knowledge on the epitaxial growth of films by vdW interactions and open up a completely new route for realizing 3D epitaxy, but also the experimental realization of its 2D limit. The DLHC structure at the initial stages of vdWE will have a major impact on the landscape of two-dimensional materials beyond single layer honeycomb such as graphene, elementary 2D (silicone, germanene, etc.), and transition metal dichalcogenides. These double-layer materials in honeycomb form, even ordinary semiconductors, such as CdTe and GaAs, will have exotic properties as yet to be discovered. Our new understanding will also impact a broad and a diverse group of research fields beyond surface science and condensed matter physics such as supramolecular chemistry, structural biology, and polymers, where vdW forces also play an important role. New principles based on these vdWE semiconductor films will impact the fabrication of electronic and optoelectronic devices used in a wide range of applications including lighting, solar energy conversion, and infrared sensing. The PIs have strong track records of integrating research, education, and outreach activities. In addition to training PhD students, they created over 90 undergraduate research projects (including many women and minority students) and co-authored more than 30 papers with undergraduates in the past 20 years. They are also active in mentoring and attracting high school students in The Empire State New Visions STEM Program to pursue science and engineering careers.