

Photoemission electron microscopy as a new tool to study the electronic properties of transition metal dichalcogenides and inhomogeneous semiconductors

Taisuke Ohta

Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, New Mexico,
United States

The energy positions of the valence and conduction electronic states with respect to the vacuum level are essential parameters to evaluate how the band gaps of semiconductors or Fermi-levels of metals line up. Such electronic structures of materials can be determined using photoemission spectroscopy (PES). PES measurements, however, remain challenging for inhomogeneous samples or materials with nano- to micro-meter lateral dimensions due to its mesoscopic probing area, typically no less than several microns. Photoemission electron microscopy (PEEM) is a cathode lens electron microscopy technique that combines photoemission imaging with spectroscopic modes of operation to provide photoemission spectra from areas less than one micron in size. Using a PEEM coupled to deep ultraviolet light sources, we studied the electronic structure of two inhomogeneous material systems: atomically-thin flakes of transition metal dichalcogenides (TMDs) supported on oxidized silicon wafers and polycrystalline cadmium telluride (CdTe) thin films for photovoltaic applications.

In the first part, we present how we revealed the band alignments and ionization energies of several TMDs (MoSe_2 , WS_2 , and MoS_2). Such information is of particular importance in predicting the performance of TMD heterostructures in devices that are useful in high performance electronics and opto-electronics. In the second part, we focus on the electronic structure variation of surface polished polycrystalline CdTe thin films with emphasis on the band alignment between the crystalline grains and grain boundaries. The impact of a key manufacturing process, the activation of the CdTe absorber layer using cadmium chloride, which drastically improves the photovoltaic power conversion efficiency, will be described in terms of the electronic structure changes. The results presented here strongly support the notion of lab-based PEEM as an emerging analytical capability to explore the electronic properties of spatially inhomogeneous materials for electronic and optoelectronic applications.

The PEEM work was performed at the Center for Integrated Nanotechnologies, an Office of Science User Facility (DE-AC04-94AL85000), with the support from CINT user program, Sandia LDRD, and a U.S. DOE-EERE SunShot BRIDGE award (DE-FOA-0000654 CPS25859). Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.