Chemical Sciences Division

Chemistry and Physics of Oxides and Wide Band-Gap Materials

The Chemistry Division has signature capabilities in epitaxial film growth and properties of oxides. Of particular strength is the ability to relate electronic, magnetic, optical, and chemical properties to film structure and composition. Our interests include ferromagnetic oxide semiconductors for spintronics, high-k dielectric epitaxial oxides on Si, and oxide/oxide heterojunctions as testbeds for fundamental studies in heterogeneous photochemistry.

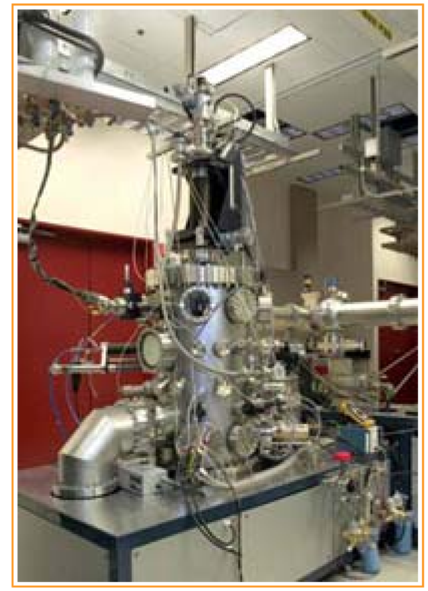

Figure 1. Growth Chamber

- 7 solid sources
- ECR oxygen plasma
- AA flux detection
- RHEED

We use oxygen plasma-assisted molecular beam epitaxy to grow crystalline films of semiconducting oxides doped with a few to several atomic percent of some magnetic dopant, such as Co or Cr. Many of these materials exhibit ferromagnetism at and above room temperature, leading to possible utility in the rapidly emerging discipline of spin electronics. Figure 1 shows the growth chamber. Figure 2 shows the photochemistry chamber for AES, MS, ultraviolet irradiation, and molecular dosing. Figure 3 shows the photoemission chamber where x-ray photoemission is done at high-energy resolution to determine valence band offsets (VBO). The VBO and associated conduction band offsets (CBO) are among the most important electronic properties of heterojunctions, which are in turn essential components in solid-state electronic devices.

At issue is the mechanism of magnetism, which is critically tied to detailed materials properties associated with dopant distribution and structure, free carrier concentration, and the possibility of secondary phase formation. We expend considerable effort conducting materials characterization measurements, such as K-edge x-ray absorption spectroscopy at the Advanced Photon Source, in order to understand the relationship between materials properties and magnetic and electronic behavior.

We use x-ray photoemission at high energy resolution to determine valence band offsets (VBO) at a variety of heterojunctions. The VBO and associated conduction band offset (CBO) are among the most important electronic properties of heterojunctions, which are in turn essential components in solid-state electronic devices. The BOs have a large influence on, among other things, the ease of carrier transport across the interface and electron-hole pair recombination velocity upon irradiation with super band gap light. Accurate BO measurements are essential to understanding the relationship between interface physical structure, electronic structure, and carrier transport. Such scientific insight is needed to solve important technological problems such as the development of a next-generation gate oxide for Si-based CMOS, which is the backbone of the computer industry. We collaborate with a number of other research groups from around the country to measure VBOs of epitaxial film systems grown at these other laboratories, in addition to performing BO measurements on systems that we grow.

We have found that interesting and potentially useful electronic structures can result at oxide/oxide interfaces and are exploiting these structures to gain fundamental insight into heterogeneous photocatalysis. In particular, we have found that the VBO sometimes exhibits noncommutative behavior, which means that its value for oxide A grown on oxide B is numerically different than that for oxide B grown on oxide A. We are using the physical separation that occurs between electrons and holes in photoexcited Fe_2O_3/Cr_2O_3 interfaces to study the photodecomposition of trimethyl acetic acid.

Figure 2. Photochemistry Chamber

- AES
- MS
- UV irradiation
- molecular dosing

Figure 3. Photoemission Chamber

- XPS - monochr. AlKα x-rays
- Scanned-angle XPD
- UPS - He I & II UV light
- LEED