

## PCSI

### Room Ballroom South - Session PCSI-4MoM

#### Surface Characterization

Moderator: Javad Shabani, New York University

11:45am **PCSI-4MoM-40 The Direct Band Gap of  $\alpha$ -Sn Investigated by Infrared Ellipsometry**, *Rigo Carrasco, C Zamarripa, S Zollner*, New Mexico State University; *J Menendez*, Arizona State University

Interest in gray tin has been revived because it is the endpoint constituent of  $\text{Ge}_{1-x}\text{Sn}_x$  alloys, which have potential applications as mid-infrared detectors and lasers,[1][2] and becomes a topological insulator or Dirac semimetal due to stress[3][4]. The band structure for gray tin is similar to Ge, but the  $\Gamma_7$  s-antibonding band, which is the conduction band in Ge, moves downward in gray tin and appears in between  $\Gamma_8^*$  and  $\Gamma_7^+$  with a negative energy  $E_0$  if we conventionally choose  $\Gamma_8^*$  as the zero energy level.

Using Fourier-transform infrared ellipsometry, we provide spectroscopic evidence about the valence band structure of  $\alpha$ -tin. The mid-infrared dielectric function of  $\alpha$ -tin grown pseudomorphically on InSb or CdTe by molecular beam epitaxy shows a strong  $E_0$  peak near 0.41 eV (Fig. 2). The peak can be attributed to the allowed intravalence band transitions from the  $\Gamma_7$  (electron-like) to the  $\Gamma_8^*$  heavy hole valence band and/or interband transitions from the  $\Gamma_7$  band to the  $\Gamma_8^*$  light "hole" conduction band. Possible sources for the strength of the peak, and its temperature dependence will be discussed. We would like to thank Dr. Arnold M. Kiefer and Stephanie Chastang for providing us the strained  $\alpha$ -tin samples.

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[3] H. Huang and F. Liu, *Phys. Rev. B* **95**, 201101 (2017).

[4] A. Barfuss, L. Dudy, M.R. Scholz, H. Roth, P. Höpfner, C. Blumenstein, G. Landolt, J.H.

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11:50am **PCSI-4MoM-41 Advanced ARPES Analyzer and Momentum Microscope KREIOS 150 – Concepts and First Results on Layered Materials and Topological Insulators**, *Thomas Schulmeyer*, SPECS-TII, Inc.

Modern ARPES analyzers provide a high degree of parallelization in data acquisition, recording hundreds of energy and angle channels simultaneously. Additionally, integrated deflectors enable users to perform angle scanning perpendicular to the analyzer's entrance slit to record (kx, ky, E) data sets without sample rotation. However, the design of conventional analyzers implies a limited acceptance angle and corresponding accessible momentum space volume. Due to the trade-off between acceptance angle and angle resolution multiple changes in sample position and lens modes are necessary during a typical high resolution ARPES experiment. The new KREIOS 150 Energy Analyzer uses an extractor zoom lens design to overcome these limitations.

This new lens provides a full solid acceptance angle with highest angular resolution. In contrast to standard ARPES measurements with conventional hemispherical analyzers, electronic structure data from and beyond the 1st Brillouin zone is recorded without any sample movement. In addition, the lens of such an instrument can work in a lateral imaging mode for microscopy as well. This enables navigation on the sample and reduces the size of the area under investigation in ARPES down to a few micrometers in diameter. This combination of large acceptance angle, high angular resolution, and small acceptance area makes this instrument the ideal tool for electronic structure studies on small samples or sample areas. The design is compact with a straight optical axis.

The capabilities of this instrument were tested at the UE 56/2 at the Bessy II synchrotron in Berlin. Specification tests show excellent angle and lateral resolution as well as small spot capability down to 2 $\mu\text{m}$  FOV. Subsequently real live samples like Graphene on Germanium were measured. Even on macroscopically rough surfaces like Graphene on NbSe<sub>2</sub> excellent ARPES and X-PEEM results could be obtained. By taking advantage of the small

spot capability of the KREIOS 150 meaningful band structure data has been recorded on such patchy samples.

Acknowledgements: We thank Yu. Dedkov (University of Shanghai, China) and M. Fonin (University Konstanz) for providing beamtime and samples for the measurements with KREIOS 150 at BESSY II.

11:55am **PCSI-4MoM-42 Investigating Relative Binding Strengths of Various Dye Attachment Chemistries at the Titania-Dye Interface in Dye-Sensitized Solar Cells**, *Gregory Smith, B Harvey, J Placzek*, Angelo State University

Dye-sensitized solar cells (DSSC) continue to be a promising area of research in our society's quest for clean and renewable energy. Typically, in these solar cells light is harvested by a dye molecule which is covalently bound to a mesoporous semiconducting material, most commonly titania. The excited electron is injected into the semiconductor and moves down to the electrode. One of the most important parts of these solar cells is the interface between the dye and the semiconductor. Optimally, the bond between dye and semiconductor should be strong, yet allow for rapid electron transport from excited dye to semiconductor. The most common chemistry for this attachment is with one or more carboxylate groups. There is a surprising lack of information about the performance of other chemistries in the literature, particularly experimental evidence. Some theoretical calculations have been performed<sup>1</sup>, but it would be very useful to have a library of the experimental performance of various attachment chemistries that could be used when considering specific dyes or in the synthesis of new dye molecules.

Here, we discuss a systematic method to compare the strength of the attachment of different chemistries to titania surfaces. To be able to directly compare chemistries, a model set of molecules were used, each 18 carbons in length capped with the group being studied. These molecules were used to form a self-assembled monolayer on a flat titania surface, then exposed to a typical solvent used in DSSCs at a slightly elevated temperature for 24 hours. The quality of the monolayer was measured before and after exposure using goniometry and ellipsometry. Table 1 shows the amount of degradation seen in each group studied. A description of the method, a comparison of the results, and how the results compare to previous theoretical studies will be included in discussion.

Terminal group:	Carboxyl	Thiol	Silane	Phosphonic acid
Degradation:	15.7 %	53.9 %	33.2 %	38.1 %

Table 1. Degradation of each monolayer after exposure to ethanol at 30°C for 24 hours.

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