

Tuesday Afternoon, November 1, 2005

Surface Science

Room 202 - Session SS1-TuA

Compound Semiconductors

Moderator: A.A. Baski, Virginia Commonwealth University

2:00pm **SS1-TuA1 Doping Semiconductor Nanocrystals**, *S.C. Erwin*, Naval Research Laboratory; *L. Zu*, U. Minnesota; *M.I. Haftel*, *A.L. Efros*, *T.A. Kennedy*, Naval Research Laboratory; *D.J. Norris*, U. Minnesota **INVITED**

Doping—the intentional introduction of impurities into a material—is fundamental to controlling the properties of bulk semiconductors. The prospect of new technologies has motivated similar efforts to dope semiconductor nanocrystals since their discovery two decades ago. Despite some successes, many of these efforts have failed, for reasons that remain mysterious. For example, individual Mn atoms can be incorporated into nanocrystals of CdS and ZnSe, but not into CdSe—despite comparable solubility limits near 50 percent in the bulk crystals. These difficulties have hindered the development of important new materials, including p- and n-type, and even magnetic, nanocrystals. Such failures have often been attributed to "self-purification," an allegedly intrinsic mechanism in nanocrystals whereby impurities are expelled to the nearby surface. Here we propose a very different view: that doping is controlled instead by the initial adsorption of impurities on the nanocrystal surface during growth. We show that impurity adsorption—and therefore doping efficiency—is determined by three main factors: the surface morphology of the nanocrystal, its overall shape, and the tendency of surfactants in the growth solution to bind the impurity. Calculated Mn adsorption energies and equilibrium shapes for several cubic and hexagonal nanocrystals lead to specific doping predictions. These are confirmed by measuring how the Mn concentration in ZnSe varies with nanocrystal size and shape. Finally, we use our predictions to incorporate individual Mn impurities into previously undopable CdSe nanocrystals. This success establishes that earlier difficulties with doping are not intrinsic, and suggests that a variety of doped nanocrystals—for applications from solar cells to spintronics—can be anticipated.

2:40pm **SS1-TuA3 Scanning Tunneling Microscopy Study of Square Manganese Tetramers on Mn₃N₂(001)**, *R. Yang*, *H.Q. Yang*, *A.R. Smith*, Ohio University

The growth of transition metal nitride layers has been a subject of significant interest due to their unique electronic, magnetic, and structural properties. We have previously investigated the growth of Mn₃N₂ on MgO(001) by molecular beam epitaxy (MBE). Mn₃N₂ is a layer-wise antiferromagnet with magnetic moments of $\sim 3 \mu_B$. Two orientations ((010) and (001)) of this structure were grown controllably on MgO(001), depending on the growth conditions. As the bulk structure corresponds to 2 layers of Mn followed by 1 layer of N in a fct arrangement, scanning tunneling microscopy (STM) shows that the (010) surface consists of row structures. These rows correspond to the Mn planes, which are perpendicular to the surface. Here we present results for the (001) surface in which the Mn planes are in the surface plane. However, this presents an interesting question regarding the epitaxial Mn₃N₂(001) growth surface, due to the Mn-N-Mn-N-Mn stacking sequence of the atomic layers in bulk. If the stacking sequence extends to the surface, then different structures should be observed on adjacent terraces. Again, these films are grown on MgO(001) substrates by MBE. STM images show smooth terraces and atomic steps. On certain of the terraces a unique and new reconstruction is seen, resolved as square Mn tetramers in a c(4x2) structural arrangement. Two domains of the tetramer reconstruction, rotated by 90 deg to each other, occur. A model is presented for this square Mn tetramer reconstruction, in which the Mn atoms of the tetramer layer belong to the Mn layer at the surface in the Mn-N-Mn-N-Mn stacking sequence. @FootnoteText@ @footnote 1@Yang et al., J. Appl. Phys. 91(3), 1053 (2002). @footnote 2@G. Kreiner, and H. Jacobs, J. Alloys and Comp. 183, 345 (1992). @footnote 3@Yang et al., Appl. Phys. Lett. 78, 3860 (2001).

3:00pm **SS1-TuA4 Investigations of Surface Reconstructions and 3D Roughening in InGaAs Films**, *L.E. Sears*, *J.M. Millunchick*, University of Michigan; *C. Pearson*, University of Michigan - Flint

The epitaxial growth of III-V semiconductors and their corresponding properties depend on the surface reconstructions and morphology of the film grown. We have found that the surface structure of In_xGa_{1-x}As alloys consists of multiple surface reconstructions

depending on the composition x . The goal of this work is to determine which reconstructions are present as a function of both composition and temperature, in order to map out the surface phase diagram for this system. For example, for In_{0.81}Ga_{0.19}As/InP grown at 503°C with an As overpressure of 2.1 ML/sec and a growth rate of 1.16 ML/sec, highly ordered regions of $\sqrt{2} \times \sqrt{2}$ coexist with more disordered regions having a (4x3) symmetry. In this case, the percentage of $\sqrt{2} \times \sqrt{2}$ covering the surface initially increases with increasing thickness, followed by a sharp decrease that corresponds to the onset of surface roughening and 3D roughening. Previous work on In_{0.27}Ga_{0.73}As/GaAs, which has a similar lattice mismatch, shows similar disordered (4x3) regions, but the highly ordered $\sqrt{2} \times \sqrt{2}$ regions have been replaced by $\sqrt{3} \times \sqrt{3}$ regions. @footnote 1@ It is postulated that the (4x3) surface reconstruction is a unique alloy structure, while the (2x4) reconstructions are enriched in In. @FootnoteText@ @footnote 1@ Millunchick JM, Riposan A, Dall B, Pearson C, and Orr BG, Surf. Sci. 550 1(1-3): 1-7 FEB 10 2004.

3:20pm **SS1-TuA5 SiO₂/GaAs Charge Build Up Induced Pinning**, *D.L. Winn*, *M.J. Hale*, University of California, San Diego

The correlation between atomic bonding sites and the electronic structure of SiO₂ on GaAs(001)-c(2x8)/(2x4), was investigated using scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), and density functional theory (DFT). At low coverage, STM images reveal that SiO₂ molecules bond Si-end down; this is consistent with Si being under-coordinated and O being fully-coordinated in SiO₂. At $\sim 5\%$ monolayer (ML) coverage, multiple bonding geometries were observed. To confirm the site assignments from STM images, DFT calculations were used to estimate the exothermicities of the different bonding geometries. However, the sites predicted to be most stable were not the most abundant sites observed in the STM experiments. To rectify the discrepancy between calculations and experiments, a total energy vs. SiO₂ chemical potential plot (i.e. SiO₂ coverage) was constructed. Once the bonding geometries were deduced, STS measurements were performed, which showed that SiO₂ pins the Fermi level at $\sim 5\%$ ML coverage. Density of state (DOS) and partial density of state (PDOS) calculations revealed that only certain bonding geometries pin the Fermi level.

3:40pm **SS1-TuA6 Phosphine and Tertiarybutylphosphine Adsorption on the Indium-Rich InP (001)-(2x4) Surface**, *R.L. Woo*, *S.F. Cheng*, *G. Chen*, *Y. Sun*, *R.F. Hicks*, University of California, Los Angeles

Phosphine (PH₃) and tertiarybutylphosphine (TBP) are widely used as the group V sources during the MOCVD growth of P-containing compound semiconductors and their alloys. The kinetics of PH₃ and TBP adsorption and phosphorus desorption from InP (001) have been studied using optical techniques and reflectance difference spectroscopy. It is found that the sticking probability of TBP decreases from 0.007 to 0.001 with increasing temperature from 420 to 520 K; whereas the sticking probability of PH₃ is approximately equal to 0.001 over the same range. In this report, we present a vibrational study of TBP and PH₃ adsorption on the indium-rich InP (001)-(2x4) surface. Both molecules form a dative bond to exposed indium atoms on the surface. A fraction of these species decompose to PH₂ or PH species with hydrogen and tertiarybutyl ligands transferring to nearby phosphorus sites. The initial datively bonded state explains the low sticking probability of these molecules, as reversible desorption competes effectively with irreversible dissociative adsorption at elevated temperatures.

Author Index

Bold page numbers indicate presenter

— C —

Chen, G.: SS1-TuA6, **1**
Cheng, S.F.: SS1-TuA6, **1**
— E —
Efros, A.L.: SS1-TuA1, **1**
Erwin, S.C.: SS1-TuA1, **1**
— H —
Haftel, M.I.: SS1-TuA1, **1**
Hale, M.J.: SS1-TuA5, **1**
Hicks, R.F.: SS1-TuA6, **1**

— K —

Kennedy, T.A.: SS1-TuA1, **1**
— M —
Millunchick, J.M.: SS1-TuA4, **1**
— N —
Norris, D.J.: SS1-TuA1, **1**
— P —
Pearson, C.: SS1-TuA4, **1**
— S —
Sears, L.E.: SS1-TuA4, **1**

Smith, A.R.: SS1-TuA3, **1**
Sun, Y.: SS1-TuA6, **1**
— W —
Winn, D.L.: SS1-TuA5, **1**
Woo, R.L.: SS1-TuA6, **1**
— Y —
Yang, H.Q.: SS1-TuA3, **1**
Yang, R.: SS1-TuA3, **1**
— Z —
Zu, L.: SS1-TuA1, **1**