Symposium UU: Real-Time Studies of Evolving Thin Films and Interfaces

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November 28 - December 2, 2010

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* Invited paper

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Granozio, G. Koster, G. Eres, C-B. Eom, N. Ingle, O.V. Kolosov, B.D. Huey, S. Hong, H. Shin
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TUTORIAL

UU/SS: Techniques for In-situ Characterization under Dynamic Conditions
Sunday, November 28, 1:30-5:00 pm
Hynes Convention Center, Room 203

This tutorial will briefly review the basic experimental aspects of various well-known characterization techniques, including transmission electron microscopy, electron diffraction, neutron and x-ray scattering, and scanning probe microscopy. From this foundation, we will provide overviews on the capabilities for adapting these characterization tools to real-time in-situ studies of materials under dynamic conditions. The overviews will include conditions such as chemical and interfacial reactions, growing surfaces, synthesis environments for nanostructures and nanoparticles, electric and magnetic fields, and electrochemical environments.

TOPICS
I. *In-situ* x-ray scattering and spectroscopy
II. *In-situ* SPM
III. *In-situ* electron microscopy

Instructors:
Eric A. Stach
Purdue University

Paul H. Fuoss
Argonne National Laboratory

Sergei Magonov
Agilent Technologies

SESSION UU1: Diffraction Techniques I
Chairs: Joel Brock and Gyula Eres
Monday Morning, November 29, 2010
Hampton (Sheraton)

8:30 AM *UU1.1
Time-Resolved X-ray Studies of the Layer-by-Layer Growth Mode of Complex-Oxide Thin-Films During Pulsed Laser Deposition. Joel D. Brock, Applied & Engineering Physics, Cornell University, Ithaca, New York.

Performing simultaneous X-Ray Reflectivity and Diffuse X-ray Scattering measurements during the deposition process, we measure the time-dependent thickness, coverage, and in-plane structure of films in the layer-by-layer growth mode. These rich data sets enable us to extract both the intra-layer and the inter-layer kinetics. Our results on the $SrTiO_3/SrTiO_3$ <001> system explicitly limit the possible role of island breakup, demonstrate the key roles played by nucleation and coarsening in Pulsed Laser Deposition, and place an upper bound on the Ehrlich-Schwoebel barrier. Using $LaAlO_3/SrTiO_3$ <001> as a model system, we demonstrate that the activation energy for diffusion varies with film thickness during the first few layers of heteroepitaxy.

9:00 AM *UU1.2
Molecular Beam Epitaxy Studied by In Situ Synchrotron X-ray and Electron Diffraction. Wolfgang Braun, Paul-Drude institute for Solid State Electronics, Berlin, Germany.

Crystal growth by molecular beam epitaxy (MBE) is characterized by a simple principle: in vacuum, atoms or molecules of only the species required to form the layer are supplied to the surface. The surface temperature is chosen such that the adatoms can move along the surface to find low-energy sites where they incorporate into the crystal. MBE is therefore ideally suited to study fundamental crystal

crystals are important in the perspective of both basics physics and their applications as catalyses. In this paper, we present an observation of the ordering and the order-disorder transition in NiPt bimetallic nano crystals using in-situ synchrotron x-ray scattering. The NiPt nano crystals of about 200 nm were formed by depositing Pt (10 nm)- Ni(10nm) thin films and annealing them rapidly to 1100°C in a high vacuum environment. The existence of the superlattice (100) Bragg peak indicated that the Ni and Pt atomic positions are ordered similar to those in bulk NiPt crystals. With increasing the temperature, the superlattice peak became more intense and sharper continuously, which was caused by the annealing of the ordered domains. The peaks started to decreases above 674°C and completely disappeared at 829° C. We also observed that NiPt bimetallic nano-crystal alloys were separated into two crystalline domains from 714°C to just below the transition temperature. In the decreasing temperature direction, however, the super lattice peak reappeared at 716°C, indicating that there is a significant hysteresis involved in the order-disorder transition. The crystal structure of the NiPt nano crystals also changed back from FCC back to L10 structure. We think that the hysteresis is related to the lattice relaxation of NiPt alloy systems.

2:45 PM UU2.5
Multiscale Simulation of Processing of New Functional Coatings by Laser Sintering of Ultrafine Composite Powders. Mikhail Krivilyov[1], Denis Danilov[2], Peter Galenko[3,1] and Vladimir Lebedev[1]; [1]Physics and Energy Engineering, Udmurt State University (UdSU), Izhevsk, Russian Federation; [2]Theoretical Biophysics, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany; [3]Institute of Materials Physics in Space, German Aerospace Center (DLR), Cologne, Germany.

Laser sintering of powder materials is a new promising technique suitable for production of a wide range of wear-resistant and corrosion-proof materials. Theoretical analysis of laser sintering of composite powders has been performed to get a robust description of rapid solidification processing leading to durable coatings. Therefore multiscale modeling of this process at the macro, meso and microscopic spatial scales was accomplished to get a closer agreement with experimental regimes. Microscopic modeling of solute segregation and phase transformation was performed using the phase field method formulated for multi component metallic alloys. Macroscopic study included modeling of transient heat transfer in a porous layer by the modified mushy zone method. According to the results of modeling, there is a distinctive difference in the final microstructure depending on the processing conditions. Under continuously operating laser significant powder compaction occurs coupled with enhanced solute redistribution driven by convection in the melted zone. Impulse laser treatment allows to achieve partial melting of the powder leaving the porous structure of the layer. This effect is potentially useful for producing chemically active/inactive coatings. Comparison between 2D and 3D simulations revealed a large deviation in the depth of the sintered zone if impulse laser processing is used. So application of the 2D model for description of the periodic thermal treatment is not appropriate if the relaxation time of the thermal field is comparable to the impulse periodicity. Phase field modeling showed the effect of solute trapping in high-speed scanning laser sintering. This happens due to high solidification velocities up to 1-5 m/s in the skin shells of the particles. Combined with the large temperature gradient up to 10^6 K/m, absolute stability of the solidification front is realized leading to chemically homogeneous composition. This effect is important in development of chemically heterogeneous coatings preserving their composite structure after sintering. Comparison of the modeling results and experimental data is performed for the Fe-Ni system.

3:30 PM *UU2.6
Three-dimensional Reciprocal Mapping and Kinematical Surface Structural Analysis by Electron Diffraction. Tadashi Abukawa, IMRAM, Tohoku University, Sendai, Japan.