

PCSI

Room Ballroom South - Session PCSI-TuM1

Oxides II

Moderator: Jaekwang Lee, Pusan National University

8:30am PCSI-TuM1-1 What Are High Entropy Ceramics and What Are They Good for?, *Alessandro Mazza*, Los Alamos National Laboratory **INVITED**

Disorder has long been a tool in changing mechanical, electronic, and other physical properties of materials. However, the amount of control is regularly limited by the enthalpy of formation for high concentrations of dopants/adatoms. As a mechanism to overcome this limitation, high entropy ceramics increase the number of elements on lattice sites – thereby lowering the overall Gibbs free energy of formation by increasing the configurational entropy of the system. Using this method, theoretical and experimental results exploring the role of disorder at this scale in manipulating spin, charge, lattice and electronic order parameters will be discussed. First, in exploring magnetism, electronic structure and valence of the high entropy ABO_3 perovskite $\text{La}_{1-x}\text{Sr}_x(\text{Cr}_{0.2}\text{Mn}_{0.2}\text{Fe}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2})\text{O}_3$. Second, in an experimental realization of extreme A-site cation disorder in $(\text{Y}_{0.2}\text{La}_{0.2}\text{Nd}_{0.2}\text{Sm}_{0.2}\text{Gd}_{0.2})\text{NiO}_3$, whose parent ternary oxides each have a large range of electronic (metal to insulator transition) and structural phase transition temperatures. In exploring these systems, it is revealed that disorder on this scale can suppress or favor certain order types, create phase frustration, and be used to design a desired phenomena not accessible by conventional materials design methods.

9:10am PCSI-TuM1-9 Atomic Layer Deposition of Cr_2O_3 : Comparing Ozone and Plasma Routes for TFTs, *Soumik Das*, Arka Sardar, imec USA; *Sean McMitchell*, IMEC Belgium; *Becky (R. L.) Peterson*, University of Michigan, Ann Arbor

Chromium(III) oxide (Cr_2O_3) is a wide-bandgap p-type semiconductor of interest for thin-film transistors (TFTs) and spintronic devices, where complementary p-type oxides are needed to pair with high-performance n-type materials such as ZnO and IGZO. Atomic layer deposition (ALD) provides the precision and conformality essential for device integration. In this work, we investigate Cr_2O_3 growth from $\text{Cr}(\text{acac})_3$ using ozone and oxygen plasma as oxidants. Plasma introduces highly reactive species that remove ligands efficiently at lower temperatures, while ozone promotes combustion-like oxidation that can enhance growth but also drive etching depending on exposure. Initial results show plasma ALD achieves sub-0.1 Å/cycle growth, though etching competes with deposition, whereas ozone requires higher substrate temperatures but produces crystalline films. Current efforts focus on optimizing precursor dosing and temperature windows to control stoichiometry and reduce defect density. Looking forward, we will fabricate and benchmark TFTs from both ozone and plasma-grown films to directly compare performance. This work will clarify how oxidant choice shapes Cr_2O_3 film quality and device behavior, guiding its use as a p-type channel in future oxide electronics and spintronics.

9:15am PCSI-TuM1-10 Correlated Oxygen States and Schottky Barrier Height in Transition Metal Oxides from First Principles, *Sohm Apte*, *Alexander Demkov*, University of Texas at Austin

Schottky barrier height (SBH) [1] that measures the potential barrier for charge transfer across a metal-semiconductor interface, is one of the central quantities for semiconductor and electro-optic devices. SBH directly affects contact resistance, rectification, leakage current, and turn-on voltage. As such, accurately predicting Schottky barrier heights from first principles is of crucial scientific and technological importance.

In the ideal Schottky-Mott picture [2], the SBH is simply defined as the difference between the work function of the metal and the electron affinity of the semiconductor. However, in real materials the presence of interface dipoles, chemical bonding, metal-induced gap states and defect-driven Fermi-level pinning, makes the determination of the SBH extremely complicated. In particular semi-local density functional theory (DFT) suffers from a self-interaction error which results in underestimated band gaps and misaligned band edges [3]. In transition-metal oxides, a common remedy is to add a Hubbard U term on the transition metal d-orbitals that form the conduction band bottom [4]. While this strategy improves bulk gaps and d-state localization, it often remains insufficient for interfaces. For several materials the calculated barrier heights significantly deviate from experimental values unless much more expensive methods like GW are employed.

Many transition metal oxides have tops of their valence bands comprise oxygen 2p states with a relatively flat dispersion. These bands have a large

effective mass and are particularly susceptible to self-interaction error, leading to a distortion in the band alignment at the interface. This observation motivates treating the oxygen 2p electrons as correlated degrees of freedom. In this work we show that introducing a Hubbard U on the oxygen 2p states systematically lowers the valence manifold, corrects the offsets, and yields quantitatively accurate barrier heights. We demonstrate this idea by choosing ten candidate oxides and constructing an interface with platinum. Platinum is a high work-function, chemically stable contact that is widely used experimentally. Importantly platinum does not readily scavenge oxygen under typical growth conditions. Beyond improving agreement, our approach is computationally efficient relative to hybrid functionals or many-body perturbation theory, making it practical for material screening and device-scale modeling.

[1] W. Schottky, Z. Phys. 113, 367 (1939)

[2] N. F. Mott, Proc. R. Soc. (London) A 171, 27 (1939)

[3] J. P. Perdew, International Journal of Quantum Chemistry 28, 497 (1985)

[4] R. T. Tung, Applied Physics Reviews 1, 011304 (2014)

9:20am PCSI-TuM1-11 Casting Metal Oxide Nanoparticle Size via Temperature-Controlled Coarsening: A Novelty in Model Picture, *Paulo Cesar de Moraes*, Catholic University of Brasilia, Brazil

The present study aims to discuss the coarsening process of freshly precipitated metal oxide nanoparticles (NPs) via short time (1-2 hours) hydrothermal treatment in mild temperature (T) range (100 to 300 °C). Transmission electron microscopy data can be used to assess the average particle diameter (D_T) of both the as-precipitated NPs and the hydrothermally treated samples at increasing temperatures. Surprisingly, the D_T versus T trend can follow a sub-linear, a linear or a super-linear behavior, depending upon the condition the diffusion process is set to take place during coarsening and the characteristics of the species diffusing in the medium. Experimental data showing different D_T versus T trends (sub-linear, linear, or super-linear) will be presented and discussed based on a physical model picture for the underlying coarsening process, which takes into account diffusion of species *in* and *out* of the NP. Moreover, the model picture predicts the limits for the sub-linear as well as the super-linear D_T versus T behavior; the former sets in as long as the thermal activated diffusion process is dominant whereas the latter may be observed for higher diffusivity values. The linear trend can be observed either in a competitive scenario involving the two above-mentioned limits (dominant thermal activated diffusion process and at higher diffusivity values) or in the absence of them. Within the limits of the model picture a linear relationship between D_T and t (coarsening time) was found, accounting for both Lifshitz and Slyozov and Wagner coarsening models (introduced in early 1960's) at relatively short times.

9:25am PCSI-TuM1-12 Coherent X-Ray Studies of Spontaneous Fluctuations in Rare Earth Nickelates, *Roopali Kukreja*, University of California at Davis **INVITED**

Rare-earth nickelates (RNiO_3) exhibit a rich interplay of electronic, magnetic, and structural phase transitions, including a metal-to-insulator transition (MIT) [1]. While these transitions have been widely studied, spontaneous fluctuations across the phase transition are mostly unexplored. Such fluctuations are increasingly recognized for enabling stochastic functionality in neuromorphic computing. Here, we employ X-ray photon correlation spectroscopy (XPCS) [2-3] to directly probe structural and magnetic fluctuations in NdNiO_3 and SmNiO_3 thin films. For NdNiO_3 , we observe a pronounced slowdown in fluctuation timescales—by an order of magnitude—near the Néel temperature, highlighting strong coupling between structural and magnetic order parameters, independent of epitaxial strain. In contrast, SmNiO_3 shows no such slowdown. Unexpectedly, wavevector-dependent measurements reveal that short-range structural fluctuations are significantly slower (by a factor of 3–5) than long-range fluctuations [4]. Our results demonstrate the power of coherent X-ray techniques in capturing nanoscale fluctuation dynamics and provide new insight into the role of fluctuations in complex oxides.

1. Middey S., Chakhalian J., Mahadevan P., Freeland J. W., Millis A. J., Sarma D. D. Physics of ultrathin films and heterostructures of rare earth nickelates. Annual Review of Materials Research 46, 305 (2016)

2. Sinha S. K., Jiang Z., Lurio L.B. X-ray photon correlation spectroscopy studies of surfaces and thin films. Advanced Materials 26, 7764 (2014)

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3. Shpyrko O.G. X-ray photon correlation spectroscopy. Journal of Synchrotron Radiation 21, 1057 (2014)
4. Zhou Hagstroem, N. et al. Critical slowdown of spontaneous fluctuations in the vicinity of metal-insulator transition in rare earth nickelates, in review (2025).

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