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Materials Genome Approach to Amorphous Metal Oxides

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The revolutionary idea of heteroepitaxial crystalline superlattices was generalized in 1989 by its author, Raphael Tsu, when he proposed to expand this concept to growing multilayers of different materials in different phases – one polycrystalline (pc), one amorphous (a). Tsu argued that the interface chemistry of the amorphous layer would allow both greater freedom of interfacial bond angles to reduce strain and greater polycrystalline component bond passivation to eliminate dangling bonds, yielding to reduced defect densities and high electron mobility. While Tsu's efforts (and those of subsequent groups) to create semiconducting superlattices in pc-Si/a-SiO2 failed owing to insufficiently flexible Si-O bond angles, a heteromorphic superlattice (HSL) has been recently realized using semiconducting pc-In2O3 layers interleaved with insulating a-MoO3 layers. Grown by precision sub-monolayer pulse-layer deposition under the same growth conditions, the HSL heterostructure with high quality validates the idea the alternating amorphous layers prevent strain accumulation in the polycrystalline layers while suppressing defect propagation across the HSL. As a result, the HSL with a 7:7 nm layer thickness exhibits a remarkable electron mobility of 71 cm2/Vs, equaling the highest quality In2O3 thin films.

In this work, the materials genome approach aids the development of metal oxide interfaces where disorder of one or both constituents is leveraged to minimize interfacial defect density while maintaining useful functionalities of both materials. Our results illustrate that bond reconfiguration and redirection of bond angles is energetically inexpensive in amorphous oxide semiconductors (AOS), ternary or quaternary oxides of post-transition metals. To navigate the large parameter space for the AOS materials, computationally-intensive ab-initio Molecular Dynamics simulations combined with comprehensive structural analysis and accurate Density-Functional calculations, have been performed for several AOS families. Integrated with systematic experimental measurements, the results provide microscopic understanding of complex relationships between the morphology, carrier generation, H intake and dynamics, and electron transport across the crystalline-amorphous transition and help derive versatile design principles for next-generation transparent amorphous semiconductors with a combination of properties not achievable in Si-based architectures.

Julia E. Medvedeva is a professor of physics and a senior investigator at Materials Research Center of Missouri University of Science and Technology. She received PhD from the Russian Academy of Science in 2002 and worked as a pre- and post-doctoral fellow at Northwestern University in Arthur Freeman's group. She joined Missouri S&T in 2005. Julia's expertise is in first-principles density functional calculations of the structural, electronic, optical, and mechanical properties of a wide range of materials, including metal oxides, nitrides, and chalcogenides, alloys, and strongly-correlated materials. She is a leading expert in the area of transparent conducting oxides. Her research work was funded by federal and private agencies as well as industry. Currently, she is Lead-PI on a materials genome grant funded by the NSF-DMREF (Designing Materials to Revolutionize and Engineer our Future) program; a co-PI on NSF-MRI (Major Research Instrumentation) grant to scale-up high-performance computational resources at Missouri S&T; and a lead theorist at Delbert E. Day Center for Glass Science and Technology.