Artificially Engineered Nanoscale Ferroelectrics

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The technical objective of our NIRT is to understand the fundamental science underlying the structural, dielectric, and optical response of artificially-engineered nanoscale ferroelectrics, which can be drastically different from that of conventional homogeneous ferroelectrics. Using "first-principles effective Hamiltonian" approaches (based on lattice Wannier functions) and Landau-Ginzburg-type phenomenological methods, we will predict the effect of one-dimensional composition and strain gradients, and mechanical and electrical boundary conditions on the appearance and stability of the spontaneous polarization in these systems and on the modifications of ferroelectric domain structures. These predictions will be compared against observations on corresponding nanostructures (made by reactive MBE) of perovskite ferroelectrics in which composition and strain are varied in one direction. The resulting films will be characterized via a combination of TEM, x-ray diffraction (including synchrotron studies), Raman spectroscopy, second harmonic generation, dielectric property measurements as a function of electric field and temperature, and piezoelectric and pyroelectric techniques and compared with corresponding theoretical predictions in order to refine our understanding of nanoscale ferroelectrics. Composition and strain gradients in ferroelectric films will be investigated as a means to incorporate new functionalities: enhanced dielectric and pyroelectric responses, as well as a variety of novel optical properties.

For over 30 years molecular beam epitaxy (MBE) has been used to build up layered semiconductor nanostructures atom-by-atom to investigate and improve our understanding of semiconductor physics and create new devices. These devices (which include laser diodes, high-performance transistors, and magnetic field sensors) have advanced healthcare, national security, communications, entertainment, and transportation-resulting in significant improvements in the quality of life for all Americans. Recent progress in research has demonstrated that this same atom-by-atom synthesis technique can be used to build up nanostructures of oxides, including ferroelectrics, with comparable nanometer-scale layering control. Since ferroelectric materials exhibit a wide variety of electrical, optical, and electromechanical properties, they are extensively used in healthcare (e.g., medical ultrasound), national defense (e.g., night vision and sonar systems), and communications (e.g., miniature capacitors for cell phones and computers). The ability to customize the layering of ferroelectric materials at the atomic-layer level opens exciting possibilities in terms of creating new functional materials that we believe can be designed (with sufficient understanding) to have exceptional properties. The improved understanding gained via this research will be applied to the development of improved (enhanced performance and smaller size) capacitors, night vision devices, and optical components. This NIRT program will also train and educate future scientists in a highly interdisciplinary research environment in a technologically-significant area of national importance.

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