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Integration of Functional Perovskites with (0001) GaN VENU VAITHYANATHAN, AARON FISHER, DARRELL G. SCHLOM, Dept. of Materials Science and Engineering, Penn State Univ., PAUL J. SHLICHTA, Crystal Research, Olympia, WA — Hybrid structures in which the functional properties of oxides can be exploited in combination with semiconductors offer exciting opportunities for devices. Perovskite oxides exhibit a wide range of functional properties motivating their integration with (0001) GaN. We used two basic criteria to select functional perovskite oxides for integration with GaN: thermodynamic stability and lattice match. Using the NIST-ICDD Crystal Data database of about 150,000 inorganic compounds, a comprehensive lattice match search was performed between all orientations of all known oxide perovskites and the (0001) face of GaN. The best lattice match was for a σ_3 boundary between the (111) pseudocubic perovskite plane and the (0001) plane of GaN. We also performed extensive thermodynamic stability calculations between all binary oxides and GaN. Our analysis led us to believe that (111) SrTiO₃ would be a good buffer layer to grow on (0001) GaN, from which the transition to one of many functional perovskite oxides could be made. Extensive attempts to integrate epitaxial (111) SrTiO₃ on (0001) GaN were, however, unsuccessful. As the surface of GaN often contains a thin Ga wetting layer, we calculated the thermodynamic stability of Ga with all binary oxides. In contrast to the thermodynamic stability of SrO in contact with GaN, SrO is found to be thermodynamically *unstable* in contact with Ga while TiO₂ is stable in contact with Ga. This is consistent with our experimental observations during the deposition of SrTiO₃ on GaN.

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