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Nano-architected GaN metamaterials with significant piezoelectric effects

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ABSTRACT

Advancements in nanoscale energy harvesting technologies have driven significant interest in piezoelectric nanogenerators. This study explores the piezoelectric behavior of nano-architected gallium nitride (GaN) metamaterials through molecular dynamics simulations, focusing on properties such as piezoelectric stress constant, piezoelectric strain constant, and specific piezopotential coefficients. Twelve different topologies from three architectural families (i.e., cubic, octahedron, and triply periodic minimal surface families) are investigated, revealing topology-dependent improvements in piezoelectric performance over bulk GaN. The effect of relative density and cell size, influenced by surface effects and surface-to-volume ratios, is systematically examined. Complementary density functional theory calculations further unravel the interaction between surface and bulk atoms, including changes in electron density and atomic bonding configurations, demonstrating the dominant influence of surface effects on piezoelectric properties at the nanoscale. Compared to other piezoelectric nanomaterials, we highlight remarkably high specific piezopotential coefficients of nano-architected GaN metamaterials. These findings underscore the potential of GaN metamaterials for developing next-generation nanogenerators and energy-harvesting devices, offering a pathway toward innovative applications in self-powered nanosensors, nanorobots, and microelectromechanical systems. The methodologies and design strategies presented here can inspire similar enhancements in other piezoelectric materials, paving the way for realizing advanced energy materials with tailored architectures.