THESIS **DEFENSE**

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Understanding Piezoelectric Nitrides by Combinatorial Methods

Date:
October 30th, 2019

Time:
10:00 AM

Place:
Hill Hall 300

Piezoelectric nitrides are technologically relevant materials, crucial for connecting today's cellular networks and positioned to enable the advanced communication networks of the future. However, new and improved piezoelectric materials are needed to deliver the performance requirements of these future networks. Here, combinatorial methods are applied in the search for new and improved piezoelectric nitride materials. In order to promote understanding of the current state of this field, a review of high-throughput methodology, nitride materials, and piezoelectric materials is presented as an introduction. A state of the art material, (Al,Sc)N, is investigated and important structure-property and composition-property relationships are illuminated by coupling computation and experiments. Further investigation, enabled by development of a new methodology, confirms a decrease in the elastic modulus with increasing scandium concentration. Chromium nitride alloying in aluminum nitride ((Al,Cr)N) is identified for similar enhancement of piezoelectric strain properties and an important structure-property relationship is investigated, and confirmed, by high-throughput experiments. A next-generation piezoelectric nitride material, $LaWN_3$, was then targeted and explored for its predicted perovskite structure and piezoelectric properties, which are both confirmed. In the process of investigating this material, the possibility of other stable nitride perovskites (ABN_3) and techniques for tuning properties through oxygen incorporation ($AB(N,O)_3$) are highlighted. In parallel to the materials studies performed here, a robust software package for combinatorial data handling was produced and distributed in order to accelerate these and future high-throughput experiments. This work documents, explores, and increases known piezoelectric nitride materials by using and advancing combinatorial methods.

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