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ScAlN: A novel piezoelectric material

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The next generation of smart phones requires bandpass filter based on acoustic wave devices working at frequencies of up to 6 GHz in order to adapt all mobile communication standards available worldwide. To enable high frequency and efficient energy transfer of these devices, highly piezoelectric and very stiff layers are required. Therefore, we have developed thin lay-ers of wurzite ScAlN showing four times the piezoelectric coefficient d33 and a similar stiff-ness in comparison to AlN used for processing surface and bulk acoustic wave devices up to date.

We present investigations of the elastic, dielectric and piezoelectric properties of aluminum scandium nitride (ScAlN) with wurtzite crystal structure by means of first-principles calcula-tions based on density functional theory added by a detailed experimental analysis of struc-tural, mechanical and polarization related effects. The goal of our approach is to use the atom-istic simulations to extract the whole set of tensor components and to confirm the theoretical prediction by experimental measurements for selected tensor coefficients of physical proper-ties relevant for piezoacoustic device design. The results presented include a detailed analysis and comparison of the calculated and the experimental data, such as the lattice coefficients, internal cell parameter, piezoelectric and stiffness matrix, Young´s and bulk modulus, dielec-tric coefficients, mass density, sound velocity as well as coupling factor for Sc-concentrations of up to x = 0.4. In addition, the theoretical and experimental data achieved and supplement-ed by information present in the literature are used to provide complete tensors for certain Sc-concentrations relevant for piezoacoustic devices. Furthermore, the dependence of a high number of physical properties are described in dependence on Sc-concentration taking nonlin-ear effects into account. By a detailed comparison to the properties and coefficients of GaAlN and InAlN alloys we point out novel properties of ScAlN in order to motivate new designs of acoustic wave devices dedicated to operate at very high frequencies.

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