Surface Acoustic Wave Propagation Characteristics in c-plane (0001) and a-plane (11-20) AlScN Thin Films

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Introduction
In order to increase the data rate in the new 5G mobile communication by a factor of ten, it is necessary to access new high-frequency bands (RF bands). Therefore, new high-speed interface devices for high-speed data transmission have to be developed which operate in the high frequency ranges up to 5 GHz. The typical devices used for this application are so called surface acoustic wave (SAW) devices. The piezoelectric performance can be significantly increased by the use of the ternary wurtzite crystal AlScN, known for its large elastic and piezoelectric constants and thus is a favorable material for applications in novel RF components.

Finite Element Method (FEM) Analysis
Acoustic properties can be computed using a 2D FEM model. Periodicity of the interdigital transducer in SAW resonators allows the use of periodic boundary condition (PBC) (see Figure 2). This leads to the Euler angles (90°, -90°, 90°) for AlScN (11-20) and (2nd) wave modes with $u$: total displacement.

SAW Resonator Model
Electro- and acoustic filters are based on acoustic resonators. In case of a SAW resonator, the electrodes are deposited on a piezoelectric material. These have a comb-shaped structure to act as an interdigital transducer as well as reflectors on both sides (see Figure 1). The resonance frequency is defined by the finger pitch of the transducer structure (see Figure 2). Only electrical signals matching frequencies can pass through this acoustic resonator. By combining several of these resonators, band pass filters for mobile communication can be realized. Typically, these devices are characterized by vector network analyzer (VNA).

Epitaxial Relationship
For the investigation of the acoustic properties of crystals, the orientations of the respective materials in the model need to be taken into account, e.g. the crystallographic axes of the thin film and the substrate have to be transformed into new coordinate systems. In this work, the orientations are represented as Euler angles [1], defined by three angles with corresponding rotations around the new axes. In a global coordinate system for the FEM study, the wave propagation direction is defined as $x$, and the surface normal as $z$. The orientations for the AlScN/Al2O3 system are transformed according to the coincidence site lattice stacking of the two crystals, resulting in the Euler angles ($0°$, $0°$, $0°$) for Al2O3(0001) and (30°, 0°, 0°) for AlScN(11-20) [2]. In the case of AlScN(11-20)/Al2O3(1-102), an ideal relationship of the a-plane for AlScN with the r-plane of Al2O3 is assumed, as illustrated in Figure 1. This leads to the Euler angles ($90°$, $-90°$, $90°$) for AlScN(11-20) and (60°, 57.3°, 90°) for Al2O3(1-102), respectively.

Comparison of AlScN Orientations
The comparison between c-plane Al0.59Sc0.41N and a-plane Al0.59Sc0.41N films with respect to $k_{eff}$ is shown in in Figure 5a. This leads to the Euler angles ($0°$, $0°$, $0°$) for Al2O3(0001) and (30°, 0°, 0°) for AlScN(11-20). In Figure 5b, the coupling of the 1st mode reaches its maximum of approximately $k_{eff} = 1.8$ % at $h_{AlScN} = 0.4$ µm, while the 2nd order waves have an increased coupling of about $k_{eff} = 4$ % at $h_{AlScN} = 0.8$ µm. In comparison, the properties of a-plane AlScN/Al2O3 are shown in Figure 5b. This leads to a good matching between the two wave modes of AlScN/Al2O3, which is advantageous for the design of new piezo-acoustic filter components.

Summary and Conclusion
The material AlScN proves to be a highly suitable candidate for future piezo-acoustic filter devices. In this work, two different orientations of wurtzite-type AlScN have been studied. For AlScN(11-20)/Al2O3(1-102) we have shown a high $k_{eff}$ and $\nu_{max}$ at the same time. The analysis of different wave modes have shown a tripling of $k_{eff}$ for the 2nd wave mode, which gives more design options for novel high frequency filters.

References