Guided propagation of surface acoustic waves in AlN and GaN films grown on 4H–SiC(0001) substrates

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I. INTRODUCTION

In the last decade, epitaxially grown GaN and AlN layers have attracted a great deal of interest in optic and electronic applications. The large band gap of GaN has been successfully applied to realize light-emitting diodes and laser diodes in the blue and ultraviolet spectral range. The large band gap is useful also for high-power and high-temperature electronic devices. Furthermore, these materials possess high sound velocities and electromechanical coupling coefficients $k^2_{\mathrm{eff}}$, making them suitable for high-frequency surface-acoustic-wave (SAW) filters, which are a critical component in communication systems. These advantageous properties of GaN and AlN imply a potential for a new type of devices, in which the optic, electronic, and acoustic features are hybridized.

At present, GaN and AlN films are typically grown on substrates like sapphire, SiC, and Si. To utilize the acoustic properties in these layered structures, one has to take into account the velocity mismatch between the overlayer and the substrate. Various SAW modes are anticipated to appear in addition to the ordinary Rayleigh mode. The most important parameter that governs the emergence of these SAW modes is the ratio between the SAW wavelength $\lambda_{\mathrm{SAW}}$ and the film thickness $d$. For $\lambda_{\mathrm{SAW}}>d$, the influence of the layered nature is, in principle, to modify the SAW velocity. On the contrary, the interference effect arising from the reflection of the acoustic waves from the substrate becomes important when $\lambda_{\mathrm{SAW}}<d$. The everlasting demand to raise the operation frequency of the SAW devices urges the reduction of $\lambda_{\mathrm{SAW}}$. Therefore, the role of the velocity mismatch becomes inevitably important in high-frequency SAW devices.

In this paper, we investigate the SAW transmission properties in GaN/SiC and AlN/SiC heterostructures. The SAW velocity in SiC (6832 m/s) is larger than the velocities in GaN (3693 m/s) and AlN (5790 m/s). The acoustic waves are hence confined in the slow-velocity films. The guiding of the SAWs gives rise to the appearance of higher-order Rayleigh modes. The variation of the velocities associated with these SAW modes when $\lambda_{\mathrm{SAW}}/d$ is changed will be compared with the prediction by theory. We will also discuss a SAW mode that propagates nearly twice as fast as the Rayleigh modes.

II. EXPERIMENT

The GaN and AlN films were grown on semi-insulating 4H–SiC(0001) substrates (this polytype of SiC is hexagonal and has four layers per unit cell) by plasma-assisted molecular-beam epitaxy. The substrate temperature was 800°C. The plasma power of 180 W (300 W) and the N$_2$ flow of 1 sccm yielded a N-limited growth rate of 0.25 $\mu$m/h (0.5 $\mu$m/h) for the AlN (GaN) films. Growth was monitored in situ by reflection high-energy electron diffraction (RHEED). The effective surface stoichiometry was adjusted to be as close to unity as possible, exploiting the recovery of the RHEED intensity upon growth interruptions. As a result, the AlN (GaN) films feature smooth surfaces with typical values for the peak-to-valley roughness of 5–15 nm (3–10 nm) and for the rms roughness of 0.5–2 nm (0.3–1 nm) over an area of $2 \times 2 \, \mu$m$^2$. The width of the (0002) x-ray rocking curve as measured by double crystal x-ray diffractometry amounts to 200–400" for the AlN films and 100–200" for the GaN films. We list in Table I the samples that we employed in our experiment. All the AlN layers were highly-

<table>
<thead>
<tr>
<th>Structure</th>
<th>Thickness ($\mu$m)</th>
<th>Carrier density ($10^{24}$ m$^{-3}$)</th>
<th>SAW direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1   AlN/SiC</td>
<td>0.25</td>
<td>...</td>
<td>[1100]</td>
</tr>
<tr>
<td>A2   AlN/SiC</td>
<td>0.5</td>
<td>...</td>
<td>[1100]</td>
</tr>
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<td>...</td>
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<td>1.25</td>
<td>...</td>
<td>[1100]</td>
</tr>
<tr>
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<td>0.9</td>
<td>[1120]</td>
</tr>
<tr>
<td>G2   GaN/SiC</td>
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<td>4.2</td>
<td>[1120]</td>
</tr>
<tr>
<td>G3   GaN/SiC</td>
<td>1.5</td>
<td>0.05</td>
<td>[1100]</td>
</tr>
</tbody>
</table>

TABLE I. Thickness of the layers for the AlN/SiC and GaN/SiC structures and carrier density for the GaN layers at room temperature. The delay lines were fabricated in the C-plane along the crystallographic directions indicated.
resistive. In contrast, the GaN layers G1 and G2 were intentionally doped, while sample G3 exhibited a background electron density of $5 \times 10^{16}$ cm$^{-3}$.

We fabricated single-finger interdigital transducers (IDTs) on the epitaxial layers by means of electron-beam lithography and lift-off techniques. The inset of Fig. 1(b) shows the scanning-electron-microscope image of one of the transducers. Here, the SAW wavelength, which is twice the period of the grating pattern, is $\lambda_{\text{SAW}} = 400$ nm. The metal gates of the IDTs are made of a 25-nm-thick evaporated Al film. A 6-nm-thick Ti film was inserted underneath the Al film to improve the adhesion of the gates to the epitaxial layers. By aligning two identical transducers, SAW delay lines were formed with a center-to-center separation of 0.5 mm. As the SAW propagation is expected to be isotropic in the C-plane of the hexagonal crystals, we stretched the delay lines along the cleavage directions of the crystals. In most of our devices, the SAWs were made to propagate along the [1100] crystallographic direction, see Table I.

The transmission and reflection characteristics of the delay lines were evaluated using an HP 8720D network analyzer. The impulse response of a delay line can be obtained by Fourier-transforming its transmission spectrum. The direct electromagnetic coupling between the transducers takes place much faster than the SAW propagation, so that the crosstalk can be isolated from the SAW transmission spectrum by filtering the corresponding component in the time domain. This gating technique has been applied for the transmission data to be presented below.

### III. Experimental Results

Figures 1(a) and 1(b) show, respectively, the transmission and reflection amplitudes in a delay line having $\lambda_{\text{SAW}}$. The inset of Fig. 1 shows a scanning-electron-microscope image of one of the transducers, which indicates the SAW wavelength of 400 nm fabricated on the AlN/SiC structure. The SAWs are generated in the [1100] crystallographic direction.

The transmission and reflection characteristics of a delay line having the SAW wavelength $\lambda_{\text{SAW}} = 0.7 \, \mu$m prepared on the AlN/SiC structure with thickness $d = 1.25 \, \mu$m. The resonances labeled $R_1$, $R_2$, and $R_3$ are associated with the first-, second-, and third-order Rayleigh modes, respectively. The higher-order Rayleigh modes can be regarded as higher-order “transverse modes” in the AlN waveguides. Analogous to the waveguide modes, the $i$th-order Rayleigh mode appears when the ratio $d/\lambda_{\text{SAW}}$ is larger than approximately $i - 1$. We note that SAWs propagate slower in sapphire than in AlN. Therefore, the guided modes are not expected to appear for AlN layers grown on sapphire.

FIG. 1. (a) Transmission and (b) reflection characteristics of a delay line having the SAW wavelength $\lambda_{\text{SAW}} = 0.7 \, \mu$m prepared on the AlN/SiC structure with thickness $d = 1.25 \, \mu$m. The number of finger pairs is 25, 41.5, 100, 114, 160, and 160 for $\lambda_{\text{SAW}} = 4.0, 2.4, 1.0, 0.7, 0.5$, and 0.43 $\mu$m, respectively. The symbols in Fig. 3 show the SAW velocity determined using the resonance frequency and $\lambda_{\text{SAW}}$. We emphasize that the data from all of the four AlN layers exhibit a universal behavior when $\lambda_{\text{SAW}}$ is normalized by $d$. We observe up to the fourth-order Rayleigh mode in our devices. The SAWs localize at the immediate vicinity of the surface over a distance of about one wavelength. Thus, the SAW velocities decrease with reducing $\lambda_{\text{SAW}}$ due to the progressive influence of the slow-velocity AlN overlayer. The variation of the

FIG. 2. Dependence of the SAW transmission on the wavelength $\lambda_{\text{SAW}}$ in the AlN/SiC structure with the film thickness $d = 1 \, \mu$m. The symbols in Fig. 3 show the SAW velocity determined using the resonance frequency and $\lambda_{\text{SAW}}$. We emphasize that the data from all of the four AlN layers exhibit a universal behavior when $\lambda_{\text{SAW}}$ is normalized by $d$. We observe up to the fourth-order Rayleigh mode in our devices. The SAWs localize at the immediate vicinity of the surface over a distance of about one wavelength. Thus, the SAW velocities decrease with reducing $\lambda_{\text{SAW}}$ due to the progressive influence of the slow-velocity AlN overlayer. The variation of the
between the measurement equipment and the IDTs.

50–100 m in our devices. Nevertheless, the long SAW wavelengths, i.e., \( \lambda_{\text{SAW}} > d \), suggest that the layered nature of the structure plays an important role for the remarkable efficiency to excite the harmonics. Owing to the large \( \lambda_{\text{SAW}} \) in this situation, a single peak was observed for the fundamental frequency. In striking contrast to this dispersion, the SAW velocities associated with the higher-order Rayleigh modes can be even faster than the SAW velocity in the SiC substrate. The higher-order Rayleigh modes are, hence, advantageous for high-frequency SAW devices.

Figure 3 contains also the data derived from the third and fifth harmonics. It should be noted that the harmonics were excited unexpectedly strongly in spite of the single-finger gates of the devices. The harmonics were observed when \( \lambda_{\text{SAW}} \) of the fundamental frequency was longer than \(~2\) \( \mu m \). In principle, the inability of exciting the harmonics for \( \lambda_{\text{SAW}} < 2 \mu m \) could result from the impedance mismatch between the measurement equipment and the IDTs. (The impedance of ITDs is determined by the aperture, which was 50–100 \( \mu m \) in our devices.) Nevertheless, the long SAW wavelengths, i.e., \( \lambda_{\text{SAW}} > d \), suggest that the layered nature of the structure plays an important role for the remarkable efficiency to excite the harmonics. Owing to the large \( \lambda_{\text{SAW}} \) in this situation, a single peak was observed for the fundamental frequency, whereas multiple peaks resulting from additional higher-order Rayleigh modes were typically observed for the harmonics.

Similar results for GaN/SiC structures are presented in Fig. 4. Five branches associated with the Rayleigh modes \( R_1 - R_5 \) are evident. The electromechanical coupling coefficient of GaN is smaller than that of AlN. The transmission amplitude in devices prepared on GaN was consequently smaller in comparison to that when the overlayers were AlN.

Nevertheless, the range of the velocity modification is more than two times wider in GaN/SiC structures than in AlN/SiC structures due to the comparatively small SAW velocity in GaN, which may be useful from an application point of view.

Although the SAW velocities are determined solely by the ratio \( d/\lambda_{\text{SAW}} \), we observe a crucial dependence of the transmission amplitude on the layer thickness. In Fig. 2, a lower-order Rayleigh mode disappears the moment a higher-order mode emerges with decreasing \( \lambda_{\text{SAW}} \). Only two peaks, as a consequence, coexist in the transmission spectra. In thicker films, however, more resonances can coexist. For instance, three peaks are seen in the transmission spectrum displayed in Fig. 1, for which \( d = 1.25 \mu m \) instead of \( d = 1.0 \mu m \) in Fig. 2. Likewise, thinner films can sustain fewer resonances simultaneously. This trend develops to such an extent that the transmission amplitude associated with the first-order Rayleigh mode was suppressed for \( d = 0.25 \mu m \) below the detection limit (~100 dB) when \( \lambda_{\text{SAW}} \) was smaller than 700 nm, whereas the second-order Rayleigh mode became strong enough for detection only when \( \lambda_{\text{SAW}} \) was less than 500 nm (not shown). No SAW transmission was, therefore, observed for 700 nm \( > \lambda_{\text{SAW}} > 400 \) nm. A possible explanation for this behavior is the small electromechanical coupling coefficient of SiC. The coupling coefficient of SiC is estimated to be one order of magnitude smaller than that of AlN (see the Appendix). Thus, the SAW excitation is expected to become difficult when the thickness of the top AlN layer is reduced. We note that the first-order Rayleigh mode seemed to disappear for \( \lambda_{\text{SAW}} < 0.7 \mu m \) irrespective of \( d \). The common critical SAW wavelength suggests that intrinsic properties of the epitaxial layers may be responsible for the disappearance.

IV. NUMERICAL RESULTS

We have carried out numerical simulations of the SAW modes in the AlN/SiC and GaN/SiC structures for under-
standing their nature. The surface of bulk hexagonal materials normally supports only one acoustic mode. This property is demonstrated by the top two curves in Fig. 5. Here, the dependence of the boundary-condition function $\Psi(f)$ on frequency $f$ is displayed for AlN and SiC. (See the Appendix for details of the numerical techniques.) The calculations were performed for $\lambda_{SAW} = 700$ nm. A surface mode corresponds to a frequency $f_R$ where $\Psi(f)$ vanishes, as indicated by the arrows, giving rise to the Rayleigh velocity $v_R = f_R \lambda_{SAW}$.

In layered structures, in contrast, $\Psi(f)$ develops multiple minima. The bottom curve in Fig. 5 displays $\Psi(f)$ for the 1.25-µm-thick AlN film on SiC (sample A4). Except for the mode labeled $R_3$, $\Psi(f)$ vanishes at the frequencies indicated by the arrows. Here, the modes polarized in the sagittal plane are denoted by $R_i$ ($i = 1, 2, \ldots$). The mode $R_1$ closely resembles the Rayleigh wave in the surface of bulk AlN, as we show below. The rest of the surface modes in Fig. 5(c), which are denoted by $L_i$, are pure shear vibrations polarized in the surface perpendicular to the propagation direction (Love-type modes). Love modes are characteristic vibrations of substrates covered by a low-velocity film. The present acoustic waveguide supports, in addition to the fundamental mode $L_1$, two overtones ($L_2$ and $L_3$) having the velocities between those of the fast transverse bulk modes of AlN and SiC.

Provided that the mass-loading effects due to the metal gratings are negligible, the velocities of the surface modes in the layered structures depend only on the ratio $d/\lambda_{SAW}$. In Figs. 3 and 4, the calculated velocities of the Rayleigh-type (solid curves) modes are shown for the AlN/SiC and GaN/SiC structures, respectively. For comparison, we also show the velocities of the lowest two Love-type modes (dotted curves) in Fig. 3. The Rayleigh-type modes indeed account for the measured resonances. The Love-type modes are piezoelectrically inactive in the AlN/SiC and GaN/SiC structures, which is the reason for their absence in the electrical measurements. Such modes, however, have been detected in Brillouin scattering experiments in GaN and AlN overlayers on silicon.

In Fig. 6, we illustrate the vertical displacement $u_3$ for the three Rayleigh modes revealed by the bottom curve in Fig. 5. Mode $R_1$ [Fig. 6(a)] has a penetration depth which is shorter than the thickness of the AlN layer and closely resembles the Rayleigh wave in bulk materials. Modes $R_2$ [Fig. 6(b)] and $R_3$ [Fig. 6(c)] are overtones of the fundamental Rayleigh mode $R_1$. The overtones are characterized by nodes in the depth-direction. The number of nodes increases for higher-order modes, reminiscent of the confined modes in waveguides.

Modes $R_1$ and $R_2$ are true surface modes as their velocities lie below those of the longitudinal bulk mode $v_T$ and the slow transverse bulk mode $v_T$ of the SiC substrate. Mode $R_3$, on the contrary, is a leaky mode as its velocity is above $v_T$. In fact, an upper limit is imposed theoretically upon the velocities of the surface modes by $v_T$. Whenever the $i$th-order Rayleigh mode emerges at $d/\lambda_{SAW} = i - 1$, its velocity takes a common initial value $v_T$. As $v_T$ is higher than the Rayleigh velocity, the higher-order modes $R_i$ ($i > 1$) can propagate even faster than the Rayleigh mode in bulk SiC.

Experimentally, some of the data indicate velocities which are considerably larger than $v_T$. Such a situation is, in principle, possible for short delay lines if the transmission loss associated with the leaky nature of the SAW modes is not critical. Nevertheless, the experimental results suggest that $v_T$ in SiC may be larger than our estimate. The latter implies that the elastic constant $c_{44}$ is larger than the value we used in our calculations as $v_T = \sqrt{c_{44}/\rho}$, with $\rho$ being the mass density, is practically determined by $c_{44}$. In fact, our value of $c_{44}$ has been chosen to achieve the best agreement with the
The fast propagation may be attributed to the “exceptional” mode, which has been predicted to exist in some layered systems.\textsuperscript{13–15} Leaky SAWs are typically strongly attenuated as the acoustic energy leaks into the bulk of the crystal. However, the attenuation vanishes when the leaky SAW degenerates into a pure bulk wave.\textsuperscript{13} The velocity of the nonattenuated leaky SAW under this special circumstance was calculated for a ZnO film prepared on SiC,\textsuperscript{14} diamond,\textsuperscript{15} or sapphire\textsuperscript{15} substrates. The SAW velocity was shown to change from the velocity of the longitudinal bulk wave $v_L$ to that of the fast transverse bulk wave $v_{T2}$ of the substrate when $d/\lambda_{SAW}$ is increased from 0 to about 0.1.

In Fig. 9, we make a comparison of the $d/\lambda_{SAW}$-dependencies of the velocity between the high-velocity mode and the guided Rayleigh modes in AlN/SiC structures. The data from $d=0.25$ and 0.5 $\mu$m layers appear to belong to an identical dispersion curve, whereas the data from $d=1.0$ $\mu$m layer apparently follow a different dispersion curve. It is thus indicated that two branches of the high-velocity mode have been observed in our devices. Although the velocity decreases with increasing $d/\lambda_{SAW}$ for both of the branches, it remains almost around $v_L$, which is not ex-
expected for the “exceptional” mode. Further experimental and theoretical works are, therefore, required to ascertain the origin of this mode. We emphasize that, regardless of the origin, the high-velocity mode provides us nearly the largest possible sound velocity from host materials as \( v_L \) in SiC is as large as the Rayleigh velocity in diamond.

VI. CONCLUSIONS

We have investigated the SAW modes in AlN and GaN layers grown on SiC substrates. The slow SAW velocity of the top layers with respect to that of the substrate results in the appearance of guided Rayleigh modes and extremely fast modes. While the velocities associated with the SAW modes are determined solely by the ratio between the SAW wave- length and the layer thickness, the transmission amplitude of each mode is found to depend crucially on the layer thickness. As long as the layer thickness is adjusted to be optimum for the desired SAW wavelengths, the present materials systems allow us to take advantage of the high SAW velocity of SiC and the large electromechanical coupling coefficient of AlN and GaN.

ACKNOWLEDGMENTS

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APPENDIX. NUMERICAL SIMULATIONS

We present in this Appendix a brief overview of the numerical techniques that we employed in our calculations. The acoustic waves are assumed to propagate along the \( x \)-direction within a surface which is normal to the \( z \)-axis. The components \( u_1 \), \( u_2 \), and \( u_3 \) of the displacement field \( \mathbf{u} = (u_1, u_2, u_3) \) are oriented along the \( x \), \( y \), and \( z \)-directions, respectively. The SAW modes in layered structures can be determined by solving the differential equation for the propagation of acoustic waves

\[
\nabla T = \rho \frac{\partial \mathbf{u}}{\partial t} \tag{A1}
\]

together with the constitutive relations

\[
T = cS - eE, \tag{A2}
\]
\[
D = eE + eS, \tag{A3}
\]

where \( T \) and \( S \) are the stress and strain tensors, respectively. The electric and displacement fields are denoted \( E = -\nabla \varphi \) and \( D \), respectively. The material parameters involved in Eqs. (A1)–(A3) are the mass density \( \rho \), the elastic constant tensor \( c \), and the piezoelectric and static dielectric tensors \( e \) and \( e_s \), respectively. We list the values of these parameters used in the calculations in Table II.

In order to calculate the SAW modes, we first determine for each layer the solutions of Eq. (A1) for a frequency \( f \) and an in-plane wave vector \( \mathbf{k}_{SAW} = (k_x, k_y) \). These solutions consist of eigenvalues of the \( z \)-component of the wave vector \( k_z \) and the mode eigenvectors \( \mathbf{v} = (u_1, u_2, u_3, \varphi) \). In the second step, the eigenvectors \( \mathbf{v} \) in adjacent layers are related to each other by imposing acoustic and electric boundary conditions at their interface. This procedure allows us to specify the eigenvectors of the surface layer in terms of those in the substrate. In the final step, we seek for surface modes, i.e., the solutions which (i) decay in the substrate and (ii) satisfy the acoustic and electric boundary conditions at the surface. These requirements can be expressed in terms of the boundary-condition function \( \Psi(f) \), which vanishes when both conditions are satisfied. The corresponding frequency \( f_R \) is the SAW frequency of the system.

In the remainder, we discuss the acoustic modes propagating in the hexagonal crystals of bulk AlN, GaN, and 4H-SiC. The velocities of the bulk modes are summarized in Table III. The acoustic velocities are isotropic for propagation in the \( C \)-plane. The modes with wave vector along the \( x \)-axis can be classified according to the symmetry relative to the

<table>
<thead>
<tr>
<th>( v_f ) (m/s)</th>
<th>( v_c ) (m/s)</th>
<th>( v_L ) (m/s)</th>
<th>( v_R ) (m/s)</th>
<th>( k_{eff}^2 ) (in ( 10^{-3} ))</th>
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<tr>
<td>GaN</td>
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(x, y)-plane, which is a mirror plane for the layered structure. The longitudinal (L) and the slow transverse (T1) modes have even symmetry with respect to the mirror plane. They are polarized in the sagittal plane, i.e., along the x- and y-directions for the L and T1 modes, respectively. Their velocities are given by \( v_L = \sqrt{c_{11}}/\rho \) and \( v_{T1} = \sqrt{c_{44}}/\rho \). The fast transverse mode \( T2 \) is uneven. Its polarization is in the plane of the surface, i.e., perpendicular to the c-axis, and the velocity is given by \( v_{T2} = \sqrt{(c_{11}-c_{12})/(2\rho)} \).

Table III also lists the velocity \( v_R \) of surface modes in the bulk materials. These Rayleigh modes have polarization in the sagittal plane and, thus, their symmetry is even with respect to the mirror operation. The Rayleigh velocities in these hexagonal crystals are lower than those of the transverse bulk vibrations (this is not the case, for instance, for piezoelectric SAWs along the [110] direction in III–V compounds). These modes, therefore, cannot be easily scattered into bulk modes.

The last column of Table III lists the effective electromechanical coupling coefficient \( k_{eff}^2 \) for the surface modes. Here, we adopt the definition of \( k_{eff}^2 \) being twice the relative change in the SAW velocity when the surface is metallized. The coupling coefficient for AlN is approximately twice as large as that of GaN. Although the coupling coefficients of AlN and GaN are larger than \( k_{eff}^2 \) of GaAs, they are an order of magnitude smaller than \( k_{eff}^2 \) of LiNbO3, which is one of the most strongly coupling piezoelectric materials. We point out that SiC is very weakly piezoelectric. Therefore, bulk SiC is not promising for SAW devices in spite of the large SAW velocity.