Surface ligand removal in atomic layer deposition of GaN using triethylgallium

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ABSTRACT

Gallium nitride (GaN) is one of the most important semiconductor materials in modern electronics. While GaN films are routinely deposited by chemical vapor deposition at around 1000 °C, low-temperature routes for GaN deposition need to be better understood. Herein, we present an atomic layer deposition (ALD) process for GaN-based on triethyl gallium (TEG) and ammonia plasma and show that the process can be improved by adding a reactive pulse, a “B-pulse” between the TEG and ammonia plasma, making it an ABC-type pulsed process. We show that the material quality of the deposited GaN is not affected by the B-pulse, but that the film growth per ALD cycle increases when a B-pulse is added. We suggest that this can be explained by the removal of ethyl ligands from the surface by the B-pulse, enabling a more efficient nitridation by the ammonia plasma. We show that the B-pulsing can be used to enable GaN deposition with a thermal ammonia pulse, albeit of x-ray amorphous films.

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I. INTRODUCTION

Gallium nitride (GaN) is a group 13-nitride semiconductor of high importance to modern electronic devices due to its optical and electronic properties. GaN has a direct and wide bandgap of 3.4 eV, a high breakdown field of 5 MV cm⁻¹, high electron mobility (theoretical limit 3200 cm²/V s), high electron saturation velocity (theoretical limit 3.15 × 10⁷ cm/s), and high thermal stability (melting point of 2500 °C).^{1,2} These properties make GaN important for high power and high-frequency electronics and optoelectronics. The fabrication of any electronic device requires the deposition of the material as a thin film. GaN thin films are typically deposited by chemical vapor deposition (CVD) at 800–1000 °C using trimethylgallium, Ga(CH₃)₃ (TMG), and ammonia, NH₃, as precursors.³ The high deposition temperatures and poor conformity of the established CVD processes for GaN are problematic for any device structure not compatible with high temperatures or that require uniform film thickness over topographically complex geometries. The deposition method of choice for such structures is atomic layer deposition (ALD). ALD processes for GaN have been developed, mainly using TMG as Ga precursor and N₂/H₂ or NH₃ plasma as N precursors.^{1,4–6} A problem with most reported ALD process for GaN is a high amount of carbon contamination, on the

order of several atomic percent.⁷ The carbon emanates from the TMG precursor, most likely due to insufficient removal of methyl groups from the surface due to the lower temperatures in ALD, 200–400 °C, compared to CVD. One route to circumvent this problem is to use Ga precursors with Ga–N bonds instead of Ga–C bonds, such as Ga[N(CH₃)₂]₃ which has been shown as a promising alternative for ALD of GaN.⁸ Another route is to slightly modify the TMG molecule to allow for easier removal of the alkyl ligands. In contrast to TMG, triethylgallium, Ga(C₂H₅)₃ (TEG), can undergo β-hydrogen elimination, a well-known, low-energy path for alkyl ligand removal. While ALD of GaN using TEG as a Ga precursor has been reported, the ligand abstraction enabled by the C–C bonds in the ligands has not been fully explored. Here, we explore how the elimination of the ethyl ligands can be enhanced for a more efficient deposition process.

II. EXPERIMENTAL DETAILS

A. Film deposition

Depositions were carried out in a Picosun R-200 atomic layer deposition tool without a load lock chamber and a operating pressure of 6 hPa. An ICP plasma was generated within a quartz tube

surrounded by a cylindrical RF coil with the substrate holder located approximately 70 cm downstream from the plasma source. ALD of GaN was done within the temperature range of 160–350 °C on 2×2 cm Si (100) with native oxide using alternative pulses of TEG and NH_3/Ar plasma, separated by N_2 purges, as precursors. TEG was kept in a stainless-steel bubbler at room temperature. N_2 (99.999%) was used as a purge gas for the whole deposition system and as a carrier gas for triethylgallium precursor delivery into the reaction chamber, while Ar (99.9997%) was used as the carrier gas for H_2 (99.999%) and NH_3 (99.999990%) precursor delivery. The N_2 , Ar, NH_3 , and H_2 gases were further purified by getter filters to further remove moisture.

Si (100) substrates were loaded and kept at a deposition temperature for at least 120 min before the growth process was started. To minimize the negative impact of atmospheric exposure during the sample loading process and to remove any water vapor adsorbed from the reactor walls upon sample loading, a 2 min NH_3/Ar (50/100 SCCM) 2800 W and 2 min N_2/Ar (50/100 SCCM) 2800 W plasma cleaning procedure was employed. This plasma pretreatment aims to reduce oxide and carbon residuals as previously reported.⁹

To study how to enhance the ethyl ligand removal from the surface, an additional pulse was added between the TEG and NH_3/Ar plasma. This made the ALD process into an ABC-type pulsed ALD process with TEG as A-pulse, the additional gas as the B-pulse and the NH_3/Ar plasma as C-pulse, similar to a previous study on ALD of aluminum nitride.¹⁰ For each set of experiments, the A-pulse was 0.3 s TEG exposure and the C-pulse was a 30 s NH_3 plasma exposure using a mixture of 50 SCCM NH_3 and 100 SCCM Ar with 2800 W plasma power. The N_2 purge was 10 s after the TEG and 6 s after the NH_3 plasma. In ABC-pulsed experiments, a 12 s B-pulse of either Ar-plasma (100 SCCM with 2000 W plasma power), H_2 gas (50 SCCM H_2 mixed with 100 SCCM Ar), or H_2 plasma (50 SCCM H_2 mixed with 100 SCCM Ar and 2000 W plasma power) was added. A 2 s N_2 purge was added after the B-pulse. Also, experiments were carried out using identical growth conditions except that the plasma during the NH_3 step was turned off to study a thermal NH_3 pulse.

B. Film characterization

The structural properties of the deposited GaN films were first analyzed by grazing incidence x-ray diffraction (GIXRD). A parallel beam x-ray mirror for Cu radiation was used as an incident beam optics, while parallel plate collimator 0.27° was used as the diffracted beam optics. The incoming beam angle, ω , was 0.5°. Data were obtained within the 2θ range of 20°–90°, which were performed using 0.05° step size and 5 s step time. Thickness and film density of the deposited films were measured by X-ray reflectometry (XRR). GIXRD and XRR were measured with a PanAnalytical X'Pert Pro. Growth per cycle (GPC) values were calculated by dividing film thicknesses by the number of ALD cycles. Surface morphologies of the GaN films were studied using a high-resolution LEO 1550 Gemini field emission scanning electron microscope (SEM). An atomic force microscope (VEECO, AFD Dimension 3100) operated under the tapping mode was used for surface topography and surface roughness. The root mean square

(RMS) surface roughness values was obtained by using the software of NANOSCOPE 5.0 to analyze the recorded results from the AFM measurements. The elemental compositions of the films were obtained using Rutherford backscattering spectrometry (RBS) and time-of-flight elastic recoil detection analyses (ToF-ERDA). The measurements were carried out in a 5-MV NEC-5SDH-2 pelletron tandem accelerator. 2 MeV $^4\text{He}^+$ ions were employed for RBS and detected at a scattering angle of 170°. Two different geometries, azimuth angle 5° + tilt angle 2° and azimuth angle 40° + tilt angle 2°, were chosen to minimize channeling effects. In addition, more suppression of the probable channeling effects was undertaken by multiple small random-angular movements around the equilibrium angles within a range of 2°. RBS spectra were fitted by SIMNRA 7.02 code.¹¹ Recoils, in ToF-ERDA, were detected at 45° angle between the primary beam and a ToF-E detector telescope in a gas ionization chamber (GIC) using a 36 MeV $^{127}\text{I}^{8+}$ beam incident at 67.5° with respect to the sample surface normal. The ToF-E detector telescope consisted of two circular carbon foils with 8 and $5 \mu\text{g}/\text{cm}^2$ thicknesses, 6 mm radius, a 0.05-msr solid angle ($\Delta\Omega$), and a flight distance of 425 mm between the foils. Utilizing a ToF-GIC setup provides the system with a good energy resolution and enhanced ion species separation in terms of mass and energy.¹² Average elemental compositions were also obtained from ToF-ERDA time-energy coincidence spectra using two different software packages, CONTES¹³ and Potku.¹⁴ Systematic uncertainties of the experiment, discussed in more detail elsewhere¹⁵ for light elements, were estimated to be a maximum of 5%–10%, whereas statistic uncertainties arisen from the number of experimental counts were $\leq 1.7\%$. However, the relative elemental concentrations were obtained with higher accuracy.^{16,17} The stopping power data required for both RBS and ERDA simulations were retrieved from SRIM2013 code.¹⁸ Chemical composition and bonding states of the films were determined by an Axis Ultra DLD instrument from Kratos Analytical x-ray photoelectron spectroscopy (XPS) with a base pressure of 1.1×10^{-9} Torr (1.5×10^{-7} Pa) and monochromatic Al K α source ($h\nu = 1486.6$ eV). Depth profiling was carried out using an Ar ion sputter beam with an acceleration voltage, spot size, and sputtering time duration of 0.5 kV, $300 \times 700 \mu\text{m}$, and 300 s, respectively. Spectra deconvolution and quantification were performed using CASA XPS software. During the peaks fitting, the C 1s peak at 285 eV was taken as a reference for all charge shift corrections.

III. RESULTS

By depositing films between 160 and 350 °C, using 0.3 s of TEG pulse, it is found that the deposition process is stable at temperatures upto, within experimental error, around 320 °C [Fig. 1(a)]. The temperature stability is regardless of which B-pulse is used, albeit the different B-pulses render different GPC. GaN deposited at 320 °C was then chosen as the deposition temperature to study the variation of GPC with TEG pulse time. The film deposition process shows a saturating behavior for TEG pulses ≥ 0.3 s, regardless of which B-pulse was used, and again the GPC values were different for the different B-pulses [Fig. 1(b)]. For both the temperature and the TEG pulse length studies, adding a B-pulse affords a higher GPC. H_2 plasma as B-pulse affords the highest

FIG. 1. Growth per cycle (GPC) for film deposition at different temperatures (a) and with different TEG pulse time (b).

GPC, Ar plasma a somewhat lower GPC, and H₂ gas shows the lowest increase in GPC. Without B-pulse, the GPC seems independent of temperature [Fig. 1(a)] between 160 and 320 °C. The GPC saturates at 0.41 Å/cycle for the TEG pulse ≥ 0.3 s [Fig. 1(b)]. Despite different GPC observed for different temperatures, the

FIG. 2. GI-XRD scans of 35 ± 3 nm thick films deposited at 320 °C with different B-pulses. All diffraction peaks can be indexed to hexagonal GaN.

impact of different B-pulses on the GPC is clear: H₂ plasma $\geq$ Ar plasma $>$ H₂ as can be seen in Fig. 1.

Stoichiometry and impurity levels of the films were measured by RBS and ERDA (Table I) on 35 ± 3 nm thick films deposited at 320 °C. As seen in Table I, all films are Ga rich and have 2–3 atomic % oxygen impurities, explained by the oxyphilic nature of GaN and the exposure to air for several days prior to ERDA/RBS measurements. The carbon impurity level is around 1 at. % in the films where no B-pulse is used or if H₂ gas is used as the B-pulse. When H₂ plasma or Ar-plasma are used as B-pulse, the carbon

TABLE I. Elemental composition from ERDA/RBS.

B-pulse	Ga (at. %)	N (at. %)	Ga/N	C (at. %)	O (at. %)	H (at. %)
None	56.5 ± 1.4	38.0 ± 1.5	1.49	1.0 ± 0.4	2.3 ± 0.5	2.2 ± 0.3
H ₂	54.5 ± 1.4	41.0 ± 1.3	1.33	1.0 ± 0.2	1.7 ± 0.3	1.8 ± 0.2
Ar-plasma	50.2 ± 1.3	44.1 ± 1.7	1.13	0.3 ± 0.1	2.9 ± 0.5	2.5 ± 0.1
H ₂ -plasma	54.0 ± 1.0	41.4 ± 1.2	1.31	0.7 ± 0.1	2.3 ± 0.3	1.6 ± 0.1

FIG. 3. HR-XPS data, Ga 3d [(a)–(d)] and N 1s [(e)–(h)] bands, of 45 ± 5 nm GaN films deposited at 320°C with different B-pulses. No B-pulse (a) and (e); Ar-plasma as B-pulse (b) and (f); H_2 gas as B-pulse (c) and (g), H_2 plasma as B-pulse (d) and (h).

level decreases to 0.7 and 0.3 at. %, respectively. The hydrogen content in the films is in the range of 1.6–2.5 at. %. It should also be noted that ERDA is a method that determines the absolute total hydrogen content¹⁹ and there is no information on whether the

hydrogen in the films is bonded, unbonded, or molecular hydrogen.

The crystal structure of 35 ± 3 nm thick films deposited at 320°C is found to be consistent with polycrystalline hexagonal GaN GIXRD (ICDD reference code: 01-073-7289) (Fig. 2). It can be noted that the B-pulse does not seem to affect the crystallinity of the films. For the ABC-type approach presented in this manuscript, the film density was found to be 5.4 g/cm^3 (no B-pulse), 5.0 g/cm^3 (Ar-plasma as B-pulse), 4.9 g/cm^3 (H_2 -gas as B-pulse), and 5.6 g/cm^3 (H_2 -plasma as B-pulse) which should be compared to 6.15 g/cm^3 for bulk GaN. Thus, the B-pulse has a slight effect on the film density.

Figure 3 shows the high-resolution XPS scans of the Ga 3d and N 1s spectral regions of GaN with 40–51 nm thick films deposited at 320°C with different B-pulses. The Ga 3d spectral region [Figs. 3(a)–3(d)] is dominated by a peak at 18.9 ± 0.5 eV, corresponding to Ga–N bonding.⁵ A minor shoulder peak at 20.5 ± 0.5 eV corresponding to Ga–O bonding.²⁰ The N 1s XPS spectral region shows a dominant peak at 396.6 ± 0.3 eV, corresponding to N–Ga bonds⁸ with a shoulder peak at 400.1 ± 0.4 eV, corresponding to N=C bonding.²¹ Auger peaks from the Ga region are also observed in the N 1s spectral region. It can be noted from Figs. 4(a)–4(e) that the B-pulse seems to reduce the Ga–O bonds in the films.

Top view scanning electron micrographs (Fig. 4) show that the 35 ± 3 nm thick films deposited at 320°C with different B-pulses have very similar morphology. According to the surface roughness analysis in our AFM measurements, the root mean square (RMS) surface roughness values were found to be 0.8 nm without B-pulse, 1.4 nm with Ar-plasma as B-pulse, 1.0 nm with H_2 gas as B-pulse, and 1.1 nm with H_2 -plasma as B-pulse.

FIG. 4. Top-view scanning electron micrographs of 35 ± 3 nm thick films deposited at 320°C with different B-pulses: no B-pulse (a), Ar-plasma as B-pulse (b), H_2 gas as B-pulse (c), and H_2 -plasma as B-pulse (d).

IV. DISCUSSION

The results presented above show that the B-pulses does not affect crystal structure, chemical bonds, or morphology of the deposited GaN films. The elemental composition of the films is only affected to a small degree by an Ar plasma as B-pulse. The most noticeable effect of the B-pulse is an increase in GPC compared to when not using a B-pulse. We hypothesize that the increase in GPC is explained by more favorable surface chemistry for the nitridation step in the deposition: After the TEG pulse, the surface will be saturated by Ga atoms bearing one or two ethyl ligands. If no B-pulse is used, the elimination of these ethyl ligands is done by the NH_3 plasma pulse which also nitridize the surface. If a B-pulse is used, the B-pulse could induce chemistry that eliminates the ethyl ligands from the surface, replacing them with other surface species that are easier to remove during the nitridation.

The gas-phase decomposition pathways of TEG at CVD conditions for deposition of gallium phosphide, 400–675 °C and 5000 Pa, has previously been studied by quantum chemical calculations.²² It was then found that TEG has two decomposition pathways in the gas phase: β -hydrogen elimination of C_2H_4 and H_2 assisted elimination of C_2H_6 . Both pathways eliminates one ethyl ligand and replaces it with a hydrogen atom on the gallium atom. The β -hydrogen elimination of the first ethyl ligand is thermodynamically favored at 400 °C, while further β -hydrogen eliminations of the other two ethyl ligands are not favored at 400 °C, but are favored at 500 °C. The H_2 assisted elimination of C_2H_6 is thermodynamically favored for all three ethyl ligands already at 400 °C.

Given these chemical pathways for the gas-phase decomposition of TEG, the B-pulses used in this study could induce ethyl eliminating surface chemistries: H_2 gas as B-pulse would favor H_2 assisted C_2H_6 elimination, an Ar-plasma would bring additional energy to the surface favoring β -hydrogen eliminations, and an H_2 -plasma as B-pulse would favor both H_2 assisted C_2H_6 elimination and β -hydrogen elimination of C_2H_4 as it brings both energy and hydrogen to the surface. These suggested surface chemical paths, summarized in Fig. 5, would all render a hydrogen-terminated surface.

The variation in GPC with the different B-pulses presented in (Fig. 1) shows that the GPC increases as: no B-pulse < H_2 gas < Ar-plasma < H_2 -plasma. It can also be seen that the most significant increase is between no B-pulse and H_2 gas as B-pulse, while the

FIG. 5. Summary of the suggested mechanisms for the enhanced removal of surface ethyl groups induced by the different B-pulses.

B-pulses bring, within experimental errors, almost the same improvement in GPC. We propose that the B-pulse serves to eliminate ethyl ligands from the surface, enabling a larger fraction of the surface to be nitridized by the NH_3 plasma since the nitridation will then to a larger extent be done on a hydrogen-terminated surface:

From the elemental composition of the films (Table I), adding a B-pulse renders a Ga/N-ratio closer to unity since the nitrogen content of the film increases. This could be an indication of more favored surface chemistry for the nitridation process with the B-pulse, which supports the above reasoning. We note that Ar-plasma as B-pulse gives the Ga/N ratio closest to 1. We speculate that this B-pulse should have the least reduction power which means that Ga(III) should have the lowest probability to be reduced to Ga(I) or Ga(0) with Ar-plasma. Since a NH_3 -plasma has very little oxidizing power for the formation of Ga(III)-nitride from Ga(I) or Ga(0) surface species. Such a reduction of Ga would be detrimental to the GaN and could lead to a Ga-rich stoichiometry. It should be noted that the carbon content of the films is not significantly affected by the B-pulses which indicate that the NH_3 -plasma can eliminate the ethyl ligands and that the B-pulse acts to prepare the surface, presumably via the formation of more reactive or less sterically hindered intermediate(s) for subsequent nitridation. However, we note that using a Ga precursor with Ga–N bonds seems to be a more favourable route to GaN with a Ga/N ratio closer to 1, as we showed in a recent publication using $\text{Ga}_2(\text{N}(\text{CH}_3)_2)_6$.⁸

FIG. 6. Summary of the GPCs measured for the different ALD processes in this study.

FIG. 7. Growth per cycle for different time of the B-pulse when a thermal NH₃ pulse is used.

Finally, ALD runs with a thermal ammonia step were conducted to study if the B-pulses render surface reactivity towards thermal NH₃. B-pulses without plasma and no B-pulse, i.e., an all-thermal ALD process with TEG and NH₃ rendered no film. Both Ar- and H₂-plasma as B-pulse lead to deposition of a film with a thermal NH₃ pulse, where the GPC was higher for the H₂-plasma, 0.2 Å/cycle, and 0.1 Å/cycle, respectively. These films were found to be x-ray amorphous and have much lower GPC compared to those made using NH₃ plasma. All GPCs obtained in this study are summarized in Fig. 6. ERDA analysis of these films showed very high oxygen content (57–75 at. %), low gallium content (12–38 at. %), and almost no nitrogen (1–5 at. %). We assign this to severe post-deposition oxidation, the films were stored in the air several days prior to ERDA analysis and interpret these contents as an indication of the very poor quality of the films.

We note that the GPC of the GaN film show a saturative behavior with the length of the B-pulse in these experiments with a thermal NH₃ pulse (Fig. 7). We have not studied saturation of the GPC with the B-pulse length for NH₃ plasma as film deposition with NH₃ plasma show much higher GPC than film deposition with thermal NH₃ given the higher reactivity of the NH₃ plasma.

V. SUMMARY

We show that the GPC in the ALD process for GaN from TEG and NH₃-plasma can be increased by adding a reactive pulse, providing energetic species, reactive species, or both to the surface, between the TEG pulse and the NH₃-plasma. The reactive pulse shows no effect on the material properties of the deposited films. We suggest that this is explained by the removal of the ethyl ligands by the reactive pulse, rendering a hydrogen-terminated surface, which is more favored for nitridation. We also show that a reactive pulse can allow for film deposition with thermal NH₃, but only affords x-ray amorphous films of very low quality.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

REFERENCES

- ¹S. Banerjee, A. A. I. Aarnink, and D. J. Gravesteijn, and A. Y. Kovalgin, *J. Phys. Chem. C* **123**, 23214 (2019).
- ²K. Park, M. A. Strosio, and C. Bayram, *J. Appl. Phys.* **121**, 245109 (2017).
- ³H. Hu, B. Zhang, L. Liu, D. Xu, Y. Shao, Y. Wu, and X. Hao, *Crystals* **10**, 141 (2020).
- ⁴C. Ozgit, I. Donmez, M. Alevli, and N. Biyikli, *J. Vac. Sci. Technol. A* **30**, 01A124 (2012).
- ⁵S. Kizir, A. Haider, and N. Biyikli, *J. Vac. Sci. Technol. A* **34**, 041511 (2016).
- ⁶M. Alevli, A. Haider, S. Kizir, S. A. Leghari, and N. Biyikli, *J. Vac. Sci. Technol. A* **34**, 01A137 (2016).
- ⁷S. Banerjee, A. J. Onnink, S. Dutta, A. A. I. Aarnink, D. J. Gravesteijn, and A. Y. Kovalgin, *J. Phys. Chem. C* **122**, 29567 (2018).
- ⁸P. Rouf, N. J. O'Brien, S. C. Buttera, I. Martinovic, B. Bakhit, E. Martinsson, J. Palisaitis, C.-W. Hsu, and H. Pedersen, *J. Mater. Chem. C* **8**, 8457 (2020).
- ⁹J. H. Kim, H. G. Choi, M.-W. Ha, H. J. Song, C. H. Roh, J. H. Lee, J. H. Park, and C.-K. Hahn, *Jpn. J. Appl. Phys.* **49**, 04DF05 (2010).
- ¹⁰P. Rouf, P. Sukkaew, L. Ojamäe, and H. Pedersen, *J. Phys. Chem. C* **124**, 14176 (2020).
- ¹¹M. Mayer, W. Eckstein, H. Langhuth, F. Schiettekatte, and U. Von Toussaint, *Nucl. Instrum. Methods Phys. Res., Sect. B* **269**, 3006 (2011).
- ¹²P. Ström, P. Petersson, M. Rubel, and G. Possnert, *Rev. Sci. Instrum.* **87**, 103303 (2016).
- ¹³K. S. Janson, *CONTES* (Uppsala University, Sweden, 2004).
- ¹⁴K. Arstila, J. Julin, M. I. Laitinen, J. Aalto, T. Konu, S. Kärkkäinen, S. Rahkonen, M. Raunio, J. Itkonen, J. P. Santanen, T. Tuovinen and T. Sajavaara, *Nucl. Instrum. Methods Phys. Res., Sect. B* **331**, 34 (2014).
- ¹⁵Y. Zhang, H. J. Whitlow, T. Winzell, I. F. Bubb, T. Sajavaara, K. Arstila, and J. Keinonen, *Nucl. Instrum. Methods Phys. Res., Sect. B* **149**, 477 (1999).
- ¹⁶M. A. Arvizu, R. T. Wen, D. Primetzhofer, J. E. Klemberg-Sapieha, L. Martinu, G. A. Niklasson, and C. G. Granqvist, *Appl. Mater. Interfaces* **7**, 26387 (2015).
- ¹⁷H. Y. Qu, D. Primetzhofer, M. A. Arvizu, Z. Qiu, U. Cindemir, C. G. Granqvist, and G. A. Niklasson, *Appl. Mater. Interfaces* **9**, 42420 (2017).
- ¹⁸J. F. Ziegler, M. D. Ziegler and J. P. Biersack, *Nucl. Instrum. Methods Phys. Res., Sect. B* **268**, 1818 (2010).
- ¹⁹U. Kroll, J. Meier, A. Shah, S. Mikhailov, and J. Weber, *J. Appl. Phys.* **80**, 4971 (1996).
- ²⁰P. Deminskyi, A. Haider, A. Ovsianitsky, A. Tsybalenko, D. Kotov, V. Matkivskyi, N. Liakhova, V. Osinsky, and N. Biyikli, in *IEEE 36th International Conference on Electronics and Nanotechnology (ELNANO)*, Kyiv 19–21 April 2016 (IEEE, Kiev, Ukraine, 2016), p. 128.
- ²¹J. T. Titantah and D. Lamoén, *Diam. Relat. Mater.* **16**, 581 (2007).
- ²²A. Stegmüller, P. Rosenowa, and R. Tonner, *Phys. Chem. Chem. Phys.* **16**, 17018 (2014).