Prediction of dislocation density in AlN or GaN films deposited on (0001) sapphire

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Abstract

The origin of threading dislocations (TDs) in nitride films is not completely understood but it is well established that they degrade the film properties. This work investigates the assumption that they arise from the interface between the film and sapphire substrate owing to small in-plane rotations between nitride domains. Bollmann's formalism is first used to determine the characteristics of dislocations at the nitride film/sapphire interface that compensate both for the parametric misfit and a small in-plane rotation of the film as frequently observed. It is shown that the dislocation density and line direction depend on the rotation angle. When islands grow and coalesce in the nucleation layer, some interfacial dislocations orientate along [0001] in the boundaries between domains and transform to so-called TDs. The amount of TDs lying in the boundaries between nitride domains is calculated as a function of the rotation angle. Estimations of TD density in the nucleation layer are deduced for a range of domain sizes and compared with experimental values of the literature.

Keywords: AlN; GaN; epitaxial growth; interfacial dislocations; threading dislocations, 0-lattice

Introduction

The performance of electronic or optoelectronic based devices prepared by thin film technology is affected by the presence of dislocations in the films. Complex mechanical or thermal stress distribution occurs during the film growth and strategies are developed to decrease the amount of dislocations during the multi-steps processing [1-3]. AlN or GaN films are mainly deposited on sapphire leading to a high parametric mismatch at the interface. The deformation at the interface is accommodated by a network of closely spaced interfacial dislocations [4-5]. In addition to interfacial dislocations, threading dislocations (TDs) aligned along the growth direction and passing through the whole thickness of the film are observed. They are assumed to come from the nucleation layer on top of the substrate [6-7]. The nucleation layer formation is inherited from the characteristics of AlN or GaN growth on sapphire, which takes place by nucleation, growth and coalescence of three dimensional islands. The islands were shown to slightly rotate from the perfect epitaxy relationship with the substrate as it was early observed in other systems [8]. These small rotations lead to angular deviations between the islands after coalescence and to the formation of dislocation arrays in the nitride films [4,5,6,7,9,10]. While some observations point out the attachment of TDs in the film to interfacial misfit dislocations [4], other works claim the disconnection between these two kinds of dislocations [11,12]. The presence of dislocation arrays at the boundary of coalesced islands is also a disputed issue [13,14].

The aim of this work is to determine the effect of island rotation in AlN or GaN layer on the generation of TDs from the film/sapphire interface using a geometrical approach. The growth and coalescence of rotated AlN or GaN islands in the nucleation layer are assumed and the density of dislocations arising from the rotation between the coalesced islands, called domains in the following, is determined. The calculation is carried out in two steps. The effect of the island rotation on the characteristics of dislocations at the film/sapphire interface is first studied using Bollmann's formalism [15,16] as it was performed for other epitaxial films [17,18]. Two starting interfacial dislocation configurations are assumed. It will be shown that the dislocation spacing and line direction vary with the in-plane rotation of the film. Then, the continuity of interfacial dislocations at the frontier between domains with different in-plane

rotation angles is studied. The characteristics of dislocations emerging from the interface in the boundaries between twisted domains are determined. Moreover, the accommodation of the angular deviation between the domains by the emerging dislocations is analysed. These data are compared with experimental evaluations of TD density in the nucleation layer from the literature.

2. Calculation of dislocation characteristics at the film/substrate interface

2.1. Method

The characteristics of the dislocation array at the film/sapphire interface depend on the parametric misfit and on the additional rotation of the film in the nucleation layer. The epitaxial relationship between the nitride film and sapphire substrate studied in this work is given by [7]:

$$(0001)_f // (0001)_s$$

$$\text{with } [01\bar{1}0]_f // [\bar{1}2\bar{1}0]_s$$

where the subscripts f and s refer to the film and sapphire, respectively. In this orientation, the parametric misfit, M, at the interface may be expressed from the difference between the magnitude of $[01\bar{1}0]_f$ and $1/3[\bar{1}2\bar{1}0]_s$ vectors which are equal to $a_f\sqrt{3}$ and a_s respectively, where a_f and a_s are the lattice parameters of the film and sapphire in the basal plane (Fig. 1).

$$M = \frac{2(a_f\sqrt{3} - a_s)}{(a_f\sqrt{3} + a_s)} \quad (1)$$

Owing to the lattice parameters of AlN ($a = 0.311$ nm, $c = 0.498$ nm) or GaN ($a = 0.319$ nm, $c = 0.518$ nm) and sapphire ($a = 0.476$ nm, $c = 1.299$ nm), the parametric misfit at room temperature is equal to +12.3% for AlN and +14.9% for GaN with sapphire as the reference.

Fig. 1: AlN (f) and sapphire (s) crystal lattices in the $(0001)_f/(0001)_s$ interface plane showing the misfit at the film/substrate interface between $[01\bar{1}0]_f$ and $1/3[\bar{1}2\bar{1}0]_s$ vectors.

This high mismatch is released in a large part by interfacial dislocations. On high resolution transmission electron microscopy (HRTEM) images of the literature, dislocations with a Burgers vector equal to $1/3\langle 2\bar{1}\bar{1}0 \rangle_f$ are observed with a spacing of about 2.1 nm for AlN [4] and 1.6 nm for GaN [5]. According to the geometry of the interface, three families of dislocations are expected with Burgers vector $a_1=1/3[2\bar{1}\bar{1}0]_f$, $a_2=1/3[\bar{1}2\bar{1}0]_f$ and $a_3=1/3[\bar{1}\bar{1}20]_f$.

The characteristics of the dislocation array are expected to change if AlN or GaN deviates from the above mutual orientation. The spacing as well as the direction of the dislocations should vary. They can be determined as a function of the misorientation using the basic equation of the O-lattice theory [15]:

$$X^0 = (I - A^{-1})^{-1} b \quad \text{if } |I - A^{-1}| \neq 0 \quad (2)$$

where A is the transformation relating the film and substrate lattices, I is the unit transformation, b is the Burgers vector of a family of dislocations, X^0 is the O-element related to b defining a place of best match between the lattices of both crystals. O-elements are calculated for all Burgers vectors of dislocations present in the interface. They can form a point lattice, or consist of parallel lines or parallel planes. Dislocation

walls are located in the form of cells around the 0-elements [15,16]. Dislocation lines are defined by the intersection of dislocation walls with the boundary plane.

In the present case, the transformation, Df, between the film and the substrate at the (0001) interface is expressed by the contraction, ε , of the film lattice in the basal plane (Fig. 1):

$$Df = \begin{pmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{where} \quad \varepsilon = \frac{as}{af\sqrt{3}} \quad (3)$$

Owing to the small difference between a_{AlN} and a_{GaN} , close values of ε are found, *i.e.* 88.4 and 86.1% for AlN and GaN, respectively.

Rotations between domains in the nucleation layer are assumed to be in-plane rotations, which is generally the dominant observed rotation mode. To simulate the island rotation in the nucleation layer, a rotation R around the $[0001]_f / [0001]_s$ axis with Θ angle ranging from -6° to 6° is considered:

$$R = \begin{pmatrix} \cos(\Theta) & -\sin(\Theta) & 0 \\ \sin(\Theta) & \cos(\Theta) & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (4)$$

The transformation A between a rotated domain and sapphire is therefore the product of R and Df:

$$A = R * Df \quad (5)$$

This equation allows the orientation and the spacing of interfacial dislocations to be determined in each domain. In the calculations, sapphire is considered to be fixed and AlN or GaN to rotate. All data were expressed in the fixed orthonormal coordinate system with X axis parallel to $[10\bar{1}0]_s$ and Y axis to $[\bar{1}2\bar{1}0]_s$ using relevant structure matrices (Fig. 1).

2.2: Interfacial dislocation characteristics

0-elements computed from eq. (5) are 0-points lying in the $(0001)_s / (0001)_f$ interface plane which form an hexagonal lattice. Both the orientation and the size of the hexagon in the interface change as a function of the rotation as illustrated in Figure 2.

Fig. 2: Illustration of the 0-point positions in the sapphire/film interface as a function of the film rotation angle: superimposition of hexagonal lattices with a side equal to a_f and $a_s/\sqrt{3}$ as illustrated in Fig. 1. (a) 0° in-plane rotation, (b) +2° rotation of AlN. The 0-points are indicated by circles. The fixed coordinate system (X,Y) used in the calculations is indicated.

According to Bollmann's approach [15] dislocation lines are drawn with respect to the 0-points. Two possibilities are considered. If hexagonal cells are drawn around 0-points, an hexagonal network of edge dislocations is obtained, each segment of the hexagon being associated with a_1 , a_2 or a_3 Burgers vector. This configuration is called dislocation set E in the following (Fig. 3a). The other alternative is an array of three families of straight dislocations associated with a_1 , a_2 or a_3 Burgers vector, lying in-between rows of 0-points. This array is called set M and consists of dislocations with 60° mixed character (Fig. 3b). In the literature, there is a consensus that dislocations at AlN/sapphire or GaN/sapphire interface correspond to set M [4]. It is a tricky question to experimentally determine which kind of dislocations really exists in the interface. In cross-sectional TEM thin foil, dislocations can reduce their line energy by rotating towards the thin foil normal. Unfortunately, in plan-view TEM specimens, the dislocation spacing is too small to image the dislocations in the studied interface. In another case, for a GaN hetero-structure associated with a small misfit, the set M consisting of three arrays of 60° mixed dislocations could be unambiguously identified [19].

Fig. 3: Schematic representation of the two dislocation sets considered in the study: disks indicate the position of the 0-points calculated for a_1 , a_2 and a_3 Burgers vectors. In (a) the set E of dislocations is an hexagonal array with segments having an edge character while in (b), the set M consists of three families of straight dislocations with mixed character.

The evolution of the 0-point positions and dislocation characteristics as a function of the AIN rotation are depicted in Fig. 4 for the set E and the set M. As the rotation angle increases clockwise, the hexagonal lattice of 0-points rotates counter clockwise and conversely. Moreover, the 0-lattice shrinks. For dislocation set E, dislocations get a mixed character and the spacing value decreases symmetrically regarding the sign of the rotation angle. Conversely, for set M, mixed dislocations transform to edge dislocations when the angle increases with a positive sign and they tend to get a screw character when the sign is negative.

Fig. 4: Evolution of the 0-point positions and dislocation characteristics as a function of the AlN film rotation in assumption of set E or M for a1, a2 and a3 dislocations. For each set, the evolution of the dislocation direction and spacing is represented by the evolution of the grey hexagon drawn for rotation angle equal to 0. As an example, the spacing of a1 dislocations (L) and the angle, α , between the X axis and a1 dislocation line are drawn for rotation angle of the film equal to 0°.

Owing to the hexagonal symmetry, similar characteristics are observed for the three dislocation families so only the results for a1 dislocations are detailed in the following. The evolution of the dislocation spacing and direction is shown in Fig. 5 for AlN (GaN). For dislocation set E, the mean dislocation spacing is equal to 2.36 nm (1.98 nm) for exact epitaxy of the film on the substrate. A slightly lower spacing value of 2.04 nm (1.72 nm) is obtained for set M due to the 60° character of the dislocations. When the film rotates, the spacing value decreases whatever the sign of the angle, a drop of about 10% is calculated for an angle of 3°. The evolution of the dislocation character with rotation angle is also pronounced and is not symmetrical regarding the sign of

the rotation angle for set M. The dislocations adopt an edge character close to 4.4° (5.5°).

Fig. 5: Evolution of a1 dislocation (a) spacing, (b) direction with rotation angle of the film for set E and M, for AlN and GaN films. In (b), α is the angle between X axis ($= [10\bar{1}0]_s$) and the dislocation line direction as illustrated in Fig. 4.

3 Calculation of threading dislocations characteristics

Previous calculations point out the influence of the in-plane film rotation on the dislocation spacing and direction in sapphire/film interface. Therefore, each island in the nucleation layer is associated with a specific interfacial dislocation array depending on the twist angle. When the islands grow and coalesce, some dislocations are expected to continue from one island to the other one, while dislocations in excess leave the interface and move to the boundaries between islands where they transform to TDs and form arrays around domains.

3.1 Method

Plan-view TEM observations detected both $(2\bar{1}\bar{1}0)$ and $(1\bar{1}00)$ prismatic habit planes for the TD arrays [7,10,20]. The orientation of the boundary between islands could be an important parameter as it affects the density of dislocations in the boundary. The example of Figure 6 depicts two domains and interfacial dislocations with same Burgers vector but a different spacing and line direction. The domains are separated either by a $(2\bar{1}\bar{1}0)$ or a $(1\bar{1}00)$ boundary. The dislocations in excess orientate in the boundary along $[0001]_f$ where they transform to TDs. The spacing S between dislocations in the boundary can be deduced from the distances between dislocations in each domain when crossing the boundary plane:

$$S = \frac{P_1 P_2}{|P_1 - P_2|} \quad (6)$$

where P_1 and P_2 are the intersections of the boundary with the periodic dislocations (Fig. 6).

Fig. 6. Drawing of slightly misoriented domains and associated interfacial dislocations with same Burgers vector. (a) Interfacial dislocations in excess from the right domain orientate along $[0001]_f$ in the boundary between domains. (b) Schematic illustrating the calculation of TD spacing according to eq. (6) (See text for meaning of P_1 and P_2).

The present study aims to calculate the density of dislocations present in the boundaries between domains with hexagonal shape assuming $(2\bar{1}\bar{1}0)$ and $(1\bar{1}00)$

prismatic habit facets. In the following, domains disoriented around $[0001]_f$ rotation axis with a positive angle are considered, where one domain is assumed to have 0° in-plane rotation (Fig. 7). As the rotation axis is parallel to the boundary plane, the boundaries between domains have a tilt character and most stable boundaries should consist of dislocations with edge character. Only the component of the Burgers vectors perpendicular to the boundary plane can compensate for the rotation, so it depends on the boundary orientation. Moreover, among dislocations, contributions opposite to the tilt deviation occur. As an example, in Fig. 7a, only dislocations with a Burgers vector component along a_1 accommodate the tilt angle. a_2 and a_3 dislocations with edge component along $-a_1$ have opposite contributions. Literature analyses of TD arrays between domains report dislocations with edge components with the same sense [7,10]. Reactions between dislocations were therefore performed in the calculations to cancel opposite components, in agreement with observations and energy criterion. Only two different kinds of dislocations remained after reaction as experimentally noticed [7,10]. These operations decrease the dislocation density in the boundary and give the lower bound of the dislocation density in the film. The upper bound, obtained by taking into account all dislocations, was also calculated.

Fig. 7. Schematic of two hexagonal domains of the film viewed along $[0001]$ direction with respective 0° and Θ in-plane rotation angle. The boundary between domains is $(2\bar{1}10)$ in (a) and $(1\bar{1}00)$ in (b). Corresponding orientations of the Burgers vectors are indicated.

The spacing of dislocations with Burgers vector a_1 , a_2 or a_3 intersecting the boundary between domains was determined in the assumption of sets E and M in the interface,

and for both kinds of boundary ($2\bar{1}\bar{1}0$) and ($1\bar{1}00$) using eq. (6). Dislocations remaining in the boundary after reaction were identified and their spacing was calculated. The density of dislocations in the boundary, d , called linear density, is deduced as the sum of the density of each kind of dislocations in the boundary which is the inverse of their spacing. Assuming that domains have a regular hexagonal shape, all boundaries of the hexagon contain the same dislocation density owing to the geometry of the system. Then, assuming that all dislocations in the film lie in the boundaries, the surface density of dislocations, D , also referred as TD density in the literature, can be expressed as a function of the side of the domains [21]:

$$D = \frac{2d}{3L} \quad \text{with } L = h\sqrt{3} \quad (7)$$

where d is the linear density of dislocations in the boundaries, h is the side of the hexagon and L is taken as the domain size; ie the island size at coalescence (Fig. 7).

The tilt angle induced by the resulting TD array was also compared with the rotation angle between domains, to evaluate if dislocations arising from the interface compensate for the rotation between domains. The rotation angle ρ between hexagonal domains accommodated by TDs in the boundary was calculated from the characteristics of the dislocations present in the boundary using Frank expression:

$$b_e = 2 S' \sin \frac{\rho}{2} \quad (8)$$

where S' is the spacing of dislocations after reaction and b_e is the Burgers vector component perpendicular to the habit plane.

3.2. Results

The characteristics of the boundary array arising from dislocation set M at the film/sapphire interface is shown in Fig. 8 for the AlN film. After cancelation of opposite Burgers vectors, only a_2 and a_3 dislocations are found in ($2\bar{1}\bar{1}0$) boundary and only a_1 and a_2 dislocations are observed for the ($1\bar{1}00$) boundary plane for the whole range of rotation angle (Fig. 8a-b). For the ($2\bar{1}\bar{1}0$) boundary the rotation angle accommodated by TDs is a little smaller than half the rotation angle between domains for angles

smaller than 4.4° . It is the opposite for the $(1\bar{1}00)$ boundary (Fig. 8c). However, a slightly larger linear density of dislocations is found for $(2\bar{1}\bar{1}0)$ boundary (Fig. 8d). It is therefore difficult to conclude which habit plane is favored in the assumption of interface set M.

Figure 8: Dislocation characteristics in the AlN film as a function of the in-plane rotation between domains for the interfacial dislocation set M. (a) Dislocation spacing after reaction for $(2\bar{1}\bar{1}0)$ boundary plane, (b) for $(1\bar{1}00)$ boundary plane, (c) tilt angle accommodated by the TD array in the boundary between domains, (d) TD linear density in $(2\bar{1}\bar{1}0)$ or $(1\bar{1}00)$ boundary.

Calculations were also carried out for interface set E (Fig. 9). About half of the in-plane rotation angle is accommodated by TDs if they lie in the $(2\bar{1}\bar{1}0)$ boundary plane while no accommodation or opposite effect occurs for the $(1\bar{1}00)$ boundary plane. The dislocation density is also slightly smaller in $(2\bar{1}\bar{1}0)$ boundary (Fig. 9b). So, for interface set M, the $(2\bar{1}\bar{1}0)$ boundary plane should be favored.

In Fig. 8d, only the lower bound of dislocation density was reported. The upper bound is given in Fig. 9b for comparison. Values are multiplied by a factor of about two or three depending on the rotation angle between domains, and remain in the same range as the ones calculated for lower bound. Moreover, rather close dislocation densities are obtained for starting interfacial dislocation sets E or M.

TD characteristics were determined for GaN films and similar results were found. Finally, TD surface densities in the films were calculated for AlN and GaN using Eq. (7) for a range of domain sizes, and values for AlN and GaN overlap as a single line for each domain size (Fig. 9c).

Figure 9. (a) Tilt angle associated with TD arrays and (b) TD linear density and upper bound of linear density (U), as a function of the in-plane rotation of domains for interfacial dislocation set E in the AlN film. (c) Comparison of the surface TD density in AlN and GaN films in case of interfacial dislocation set M.

4. Discussion

TD density values are available in the literature both for AlN or GaN films. They arise from direct measurements in transmission electron microscopy (TEM) or they are derived from models using XRD data [22]. In this study, only experimental values

measured at the top of the nucleation layer can be used for comparison with calculations. In GaN films, density values between $5 \times 10^9 \text{ cm}^{-2}$ to $5 \times 10^{10} \text{ cm}^{-2}$ for domain sizes evaluated in the 200-500 nm range were found [7,23,24]. Close values between 5 to $8 \times 10^{10} \text{ cm}^{-2}$ were determined in AlN films for domains between 20 to 50 nm [4,10,20,25,26]. The mean rotation angle between domains together with the domain size and the dislocation density are usually not available for the same film in the literature. TEM measurements of the rotation angle between domains indicate large variations of rotation angles, as angles smaller than 1.3° or 2.9° in AlN [10,20] or smaller than 0.3° or 3° in GaN [6,7]. The experimental densities were therefore compared with values calculated for the observed rotation angles and domain size range. Calculations replicate quantitatively the literature data (Fig. 10).

Figure 10. TD density calculated as a function of the rotation angle between domains for domain size (a) in the 100-500 nm range for GaN (b) in the 20-100 nm range for AlN (M set and $(2\bar{1}\bar{1}0)$ boundary plane). Domain sizes in bold relate to experimentally observed sizes and grey area delineates experimental TD density values recorded at the level of the nucleation layer.

As a comparison, the assumption of low angle boundaries fully accommodating the rotation between domains was also explored, assuming no link between interfacial dislocations and TDs dislocations. The calculation leads to dislocation densities about twice the previous results which are still in the range of the observed values. However, the hypothesis of low angle boundaries disconnected from film/sapphire interface

seems very unlikely looking at the effect of domain rotation on the interfacial dislocation characteristics.

When dislocations between domains arise from the interface, the tilt angle between domains is only partly compensated by dislocations. It results in a large amount of disorder at the boundaries between domains. Disorder in nucleation layers seems however favourable when a growth in two steps is used [1,27]. Compared with AlN, GaN has a cubic structure at low temperature and transforms to an hexagonal structure on heating. This leads to the formation of numerous stacking faults in the nucleation layer [14]. They influence the defect content of the nucleation layer for GaN films and seem to have a positive effect on the final dislocation content of the films [20].

A two-stage growth process is usually performed to reduce the dislocation density of the films. It is observed that many TDs of the nucleation layer bend at the interface between the nucleation layer and the growth layer. In the growth layer, the number of domains decreases and the film grows with preferentially 0° in-plane rotation [24,28]. It is not known if new domains are nucleated above the nucleation layer or if a reduced number of domains grow from the nucleation layer. The bending of the dislocations at the boundary between the nucleation layer and the growth layer is usually attributed to the stress distribution in the film [3]. It could also be related to the misorientation between the nucleation and the growth layers. Assuming a boundary plane parallel to (0001) between these layers, the boundary has a twist character which can be accommodated by screw or mixed a_1 , a_2 or a_3 dislocations. The bending dislocations should contribute to the elastic equilibrium of this boundary.

5 Conclusion

In this work, the characteristics of dislocations in the film/sapphire interface were determined using the O-lattice approach for a range of misorientation angles of AlN or GaN films with the assumption of two interfacial dislocation sets. Set E with pure edge dislocations for 0° in-plane rotation gives rise to larger dislocation spacing than set M with mixed character, whatever the rotation angle. The spacing between dislocations at the film/sapphire interface varies with the in-plane rotation of the film. A slightly

smaller spacing is found for GaN owing to the larger parametric misfit with sapphire. A significant variation of the dislocation direction also occurs for small rotation angles.

As the interfacial dislocation content depends on the in-plane rotation of the film, some dislocations have to stop at the boundary between domains where they transform into TDs. These TDs were quantified assuming $(2\bar{1}\bar{1}0)$ or $(1\bar{1}00)$ boundaries between domains as observed in the literature. The nature of the interfacial dislocation set has little impact on the TD density. $(2\bar{1}\bar{1}0)$ TD array compensates about half of the in-plane rotation between domains unlike $(1\bar{1}00)$ TD array but can contain a higher amount of dislocations. This probably explains why both $(2\bar{1}\bar{1}0)$ and $(1\bar{1}00)$ kinds of boundaries are observed in the films.

The TD density in the film was determined for a range of domain sizes as a function of the in-plane rotation between domains. Calculation indicate similar values for AlN and GaN and are in agreement with experimental densities measured at the level of the nucleation layer. The correlation between experiments and calculation supports the hypothesis that TDs are related to the rotation between domains in the nucleation layer.

This approach can be used to predict the effect of domain size, shape, and in-plane rotation of the film on the TD density regarding the substrate/film interface mismatch. It could help to design the substrate geometry in order to reduce the TD density in the films.

Compliance with Ethical Standards:

Conflict of Interest: The authors declare that they have no conflict of interest.

References

[1] Balaji M, Claudel A, Fellmann V, Gélard I, Blanquet E, Boichot R, Coindeau S, Roussel H, Pique D, Baskar K, Pons M (2012) Significance of initial stages on the

epitaxial growth of AlN using high temperature halide chemical vapor deposition. *Physica status solidi c* 9 (3-4):511-514. doi: 10.1002/pssc.201100357

[2] Chubarov M, Mercier F, Lay S, Charlot F, Crisci A, Coindeau S, Encinas T, Ferro G, Reboud R, Boichot R (2017) Growth of aluminum nitride on flat and patterned Si (111) by high temperature halide CVD. *Thin Solid Films* 623:65-71. doi:10.1016/j.tsf.2016.11.045

[3] Jiang K, Sun X, Ben J, Jia Y, Liu H, Wang Y, Wu Y, Kai C, Li D (2018) The defect evolution in homoepitaxial AlN layers grown by high-temperature metal-organic chemical vapor deposition. *CrystEngComm* 20 (19):2720-2728

[4] Kehagias T, Komninou P, Nouet G, Ruterana P, Karakostas T (2001) Misfit relaxation of the AlN/Al₂O₃ (0001) interface. *Physical Review B* 64 (19):195329

[5] Kwon YB, Je JH, Ruterana P, Nouet G (2005) On the origin of a-type threading dislocations in GaN layers. *Journal of Vacuum Science & Technology A* 23 (6):1588-1591

[6] Qian W, Skowronski M, Degraef M, Doverspike K, Rowland LB, Gaskill DK (1995) Microstructural Characterization of Alpha-GaN Films Grown on Sapphire by Organometallic Vapor-Phase Epitaxy. *Appl Phys Lett* 66 (10):1252-1254. doi:10.1063/1.113253

[7] Ning XJ, Chien FR, Pirouz P, Yang JW, Khan MA (1996) Growth defects in GaN films on sapphire: The probable origin of threading dislocations. *Journal of Materials Research* 11 (3):580-592

[8] Jesser WA, Kuhlmann-Wilsdorf D (1968) Angular distribution of epitaxial gold nuclei on a molybdenite substrate as a function of substrate temperature and nucleus size. *Acta Metallurgica* 16:1325-33

[9] Heffelfinger JR, Medlin DL, McCarty KF (1999) On the initial stages of AlN thin-film growth onto (0001) oriented Al₂O₃ substrates by molecular beam epitaxy. *Journal of Applied Physics* 85 (1):466-472

[10] Tokumoto Y, Shibata N, Mizoguchi T, Sugiyama M, Shimogaki Y, Yang J-S, Yamamoto T, Ikuhara Y (2008) High-resolution transmission electron microscopy (HRTEM) observation of dislocation structures in AlN thin films. *J Mater Res* 23 (8):2188-2194

[11] Oliver RA, Kappers MJ, Humphreys CJ (2006) Insights into the origin of threading dislocations in GaN/Al₂O₃ from atomic force microscopy. *Appl Phys Lett* 89 (1):011914

[12] Moram MA, Oliver RA, Kappers MJ, Humphreys CJ (2009) The Spatial Distribution of Threading Dislocations in Gallium Nitride Films. *Advanced Materials* 21:3941-3944

[13] Narayanan V, Lorenz K, Kim W, Mahajan S (2001) Origins of threading dislocations in GaN epitaxial layers grown on sapphire by metalorganic chemical vapor deposition. *Appl Phys Lett* 78 (11):1544-1546

- [14] Narayanan V, Lorenz K, Kim W, Mahajan S (2002) Gallium nitride epitaxy on (0001) sapphire. *Philosophical Magazine A* 82 (5):885-912.
- [15] Bollmann W (1970) *Crystal defects and crystalline interfaces*. Springer-Verlag, Berlin
- [16] Bollmann W (1972) The basic concepts of the O-lattice theory. *Surface Science* 31:1-11
- [17] Dakshinamurthy S, Rajan K (1991) An affine transformation description of epitaxial heterostructures. *Journal of Electronic Materials* 20 (7):747-752
- [18] McIntyre PC, Maggiore CJ, Nastasi M (1997) Epitaxy of Pt thin films on (001) MgO-I. Interface energetics and misfit accommodation. *Acta Materialia* 45 (2):869-878
- [19] Li QT, Minj A, Chauvat MP, Chen J, Ruterana P (2017) Interface dislocations in In_xGa_{1-x}N/GaN heterostructures. *physica status solidi (a)* 214 (4):1600442. doi:10.1002/pssa.201600442
- [20] Su XJ, Huang J, Zhang JP, Wang JF, Xu K (2019) Microstructure and influence of buffer layer on threading dislocations in (0001) AlN/sapphire grown by hydride vapor phase epitaxy. *Journal of Crystal Growth* 515: 72-77. <https://doi.org/10.1016/j.jcrysgro.2019.03.012>
- [21] Gay P, Hirsch PB, Kelly A (1953) The estimation of dislocation densities in metals from X-ray data. *Acta Metallurgica* 1:315-9
- [22] Lee SR, West AM, Allerman AA, Waldrip KE, Follstaedt DM, Provencio PP, Koleske DD, Abernathy CR (2005) Effect of threading dislocations on the Bragg peakwidths of GaN, AlGaIn, and AlN heterolayers. *Appl Phys Lett* 86 (24):241904
- [23] Heying B, Wu XH, Keller S, Li Y, Kapolnek D, Keller BP, DenBaars SP, Speck JS (1996) Role of threading dislocation structure on the x-ray diffraction peak widths in epitaxial GaN films. *Appl Phys Lett* 68 (5):643-645
- [24] Wu XH, Fini P, Tarsa EJ, Heying B, Keller S, Mishra UK, DenBaars SP, Speck JS (1998) Dislocation generation in GaN heteroepitaxy. *Journal of Crystal Growth* 189-190:231-243
- [25] Claudel A, Fellmann V, Gélard I, Coudurier N, Sauvage D, Balaji M, Blanquet E, Boichot R, Beutier G, Coindeau S, Pierret A, Attal-Trétout B, Luca S, Crisci A, Baskar K, Pons M (2014) Influence of the V/III ratio in the gas phase on thin epitaxial AlN layers grown on (0001) sapphire by high temperature hydride vapor phase epitaxy. *Thin Solid Films* 573:140-147
- [26] Boichot R, Chen D, Mercier F, Baillet F, Giusti G, Coughlan T, Chubarov M, Pons M (2017) Epitaxial Growth of AlN on (0001) Sapphire: Assessment of HVPE Process by a Design of Experiments Approach. *Coatings* 7:136. doi:10.3390/coatings7090136
- [27] Balaji M, Claudel A, Fellmann V, Gélard I, Blanquet E, Boichot R, Pierret A, Attal-Trétout B, Crisci A, Coindeau S, Roussel H, Pique D, Baskar K, Pons M (2012) Effects of

AlN nucleation layers on the growth of AlN films using high temperature hydride vapor phase epitaxy. *Journal of Alloys and Compounds* 526:103-109

[28] Su X, Zhang J, Huang J, Zhang J, Wang J, Xu K (2017) Defect structure of high temperature hydride vapor phase epitaxy-grown epitaxial (0001) AlN/sapphire using growth mode modification process. *Journal of Crystal Growth* 467:82-87