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INTERNATIONAL STANDARD

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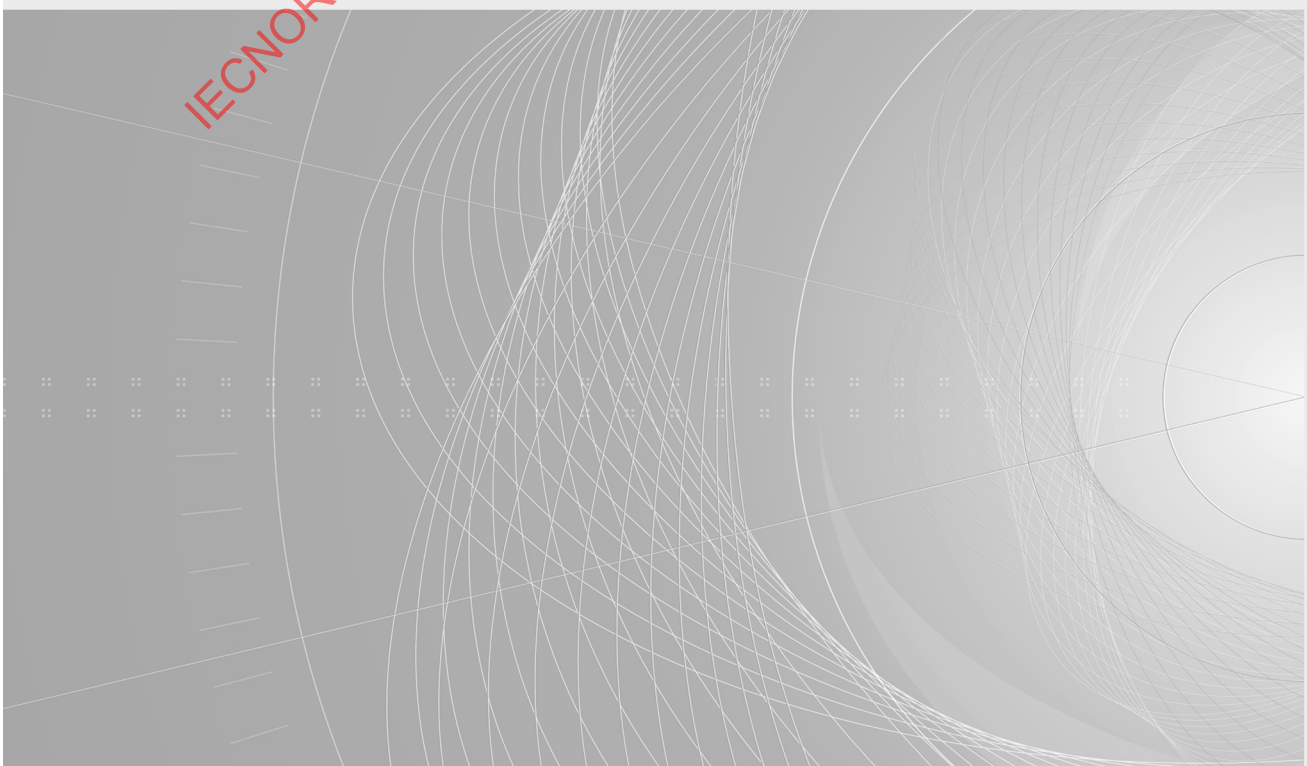
Semiconductor devices – Classification of defects in gallium nitride epitaxial film on silicon carbide substrate



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SEMICONDUCTOR DEVICES – CLASSIFICATION OF DEFECTS IN GALLIUM NITRIDE EPITAXIAL FILM ON SILICON CARBIDE SUBSTRATE

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The text of this International Standard is based on the following documents:

FDIS	Report on voting
47/2687/FDIS	47/2693/RVD

Full information on the voting for its approval can be found in the report on voting indicated in the above table.

The language used for the development of this International Standard is English.

This document was drafted in accordance with ISO/IEC Directives, Part 2, and developed in accordance with ISO/IEC Directives, Part 1 and ISO/IEC Directives, IEC Supplement, available at www.iec.ch/members_experts/refdocs. The main document types developed by IEC are described in greater detail at www.iec.ch/standardsdev/publications.

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- reconfirmed,
- withdrawn,
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- amended.

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INTRODUCTION

Gallium nitride (GaN) as a representative of the wide band gap semiconductors has outstanding properties, such as wide band gap, high critical electric field, high electron saturation drift velocity, and good resistance to corrosion and radiation. Owing to these properties, GaN can bring significant improvements to electronic devices, such as high-voltage, high-frequency, and high-power, which will be widely used in wireless communication base stations, radars, automotive electronics, aerospace, the nuclear industry, and military electronics.

To date, the development of GaN epitaxial film and related devices is hindered by high cost, low yield, and poor reliability. Among them, the defects in GaN epitaxial film, which closely related to device reliability, are especially serious.

There are various defects found in GaN epitaxial film on silicon carbide (SiC) substrate. In addition, global researchers have not established a uniform definition and classification criterion for defects in GaN epitaxial film yet. Thus, it is essential to establish a set of international standards for GaN epitaxial film on SiC substrate, which will benefit the development of GaN epitaxial film and related devices.

To define and classify defects in GaN epitaxial film on SiC substrate, a new international standard is proposed. The main contents of this document are listing and illustrating the definition and classification of defects in GaN epitaxial film on SiC substrate, providing reference for future GaN-related research and device manufacture.

SEMICONDUCTOR DEVICES – CLASSIFICATION OF DEFECTS IN GALLIUM NITRIDE EPITAXIAL FILM ON SILICON CARBIDE SUBSTRATE

1 Scope

This International Standard gives guidelines for the definition and classification of defects in GaN epitaxial film grown on SiC substrate. They are identified and described on the basis of examples, mainly by schematic illustrations, optical microscope images, and transmission electron microscope images for these defects. This document covers only defects in as-grown GaN epitaxial film on SiC substrate and does not include defects caused by subsequent processes.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

- IEC Electropedia: available at http://www.electropedia.org/
- ISO Online browsing platform: available at http://www.iso.org/obp

3.1
Gallium nitride
GaN
compound semiconductor crystal composed of gallium and nitrogen

3.2
substrate
material on which epitaxial layer is deposited

[SOURCE: IEC 63068-1:2019, 3.9, modified – "Homoepitaxial" has been replaced by "epitaxial".]

3.3
Silicon carbide
SiC
semiconductor crystal composed of silicon and carbon, which exhibits a large number of polytypes such as 4H and 6H

Note 1 to entry: A symbol like 4H gives the number of periodic stacking layers (2, 3, 4,…) and the crystal symmetry (H=hexagonal) of each polytype.

[SOURCE: IEC 63068-1:2019, 3.1, modified – Polytype of 3C has been deleted.]

3.4
4H-SiC
SiC crystal showing a hexagonal symmetry, in which four Si-C layers are periodically arranged along the crystallographic c-axis

Note 1 to entry: The crystal structure of 4H-SiC is similar to wurtzite with a unit cell having four periodical occupied sites along the <0001> directions.

[SOURCE: IEC 63068-1:2019, 3.3]

3.5
6H-SiC
SiC crystal showing a hexagonal symmetry, in which six Si-C layers are periodically arranged along the crystallographic c-axis

Note 1 to entry: The crystal structure of 6H-SiC is similar to wurtzite with a unit cell having six periodical occupied sites along the <0001> directions.

[SOURCE: IEC 63068-1:2019, 3.4]

3.6
crystal
monocrystalline material

[SOURCE: IEC 63068-1:2019, 3.11]

3.7
crystal direction
direction, denoted as [*uvw*], representing a vector direction in multiples of the basis vectors describing the *a*-, *b*- and *c*-axis

Note 1 to entry: In GaN showing a hexagonal symmetry, four-digit indices [*uvtw*] are frequently used for crystal directions.

Note 2 to entry: Families of symmetrically equivalent directions are written by <*uvw*> and <*uvtw*> for hexagonal symmetries.

[SOURCE: IEC 63068-1:2019, 3.6, modified – In Note 1 to entry, "4H-SiC" has been replaced by "GaN" and "cubic" has been deleted.]

3.8
lattice
specific form of atomic arrangement within the crystal

3.9
basal plane
plane perpendicular to the crystallographic *c*-axis, which is parallel to <0001>, in a hexagonal crystal

[SOURCE: IEC 63068-1:2019, 3.13, modified – The expression "which is parallel to <0001>", has been added.]

3.10
defect
interruption of crystallinity

Note 1 to entry: Defect in GaN epitaxial film on SiC substrate including point defect, linear defect, volume defect, surface defect and the others.

3.11
point defect
crystal defect that occurs at or around a single lattice site, such as vacancy, interstitial, substitutional defect and point defect complex

3.12
surface defect
morphological irregularity on the epitaxial layer surface, not associated with extended defects in the underlying layer

[SOURCE: IEC 63068-1:2019, 3.37, modified –"homoepitaxial" has been replaced by "epitaxial".]

3.13
Schottky defect
vacancy created at the original site when an atom escapes from its lattice site to the surface of the crystal

3.14
Frenkel defect
vacancy created at the original site when an atom delivers from its lattice site to an interstitial site of the crystal

3.15
shallow donor
defect which has a band emission below the conduction band but above 1/2 band gap

3.16
shallow acceptor
defect which has a band emission above the valence band but below 1/2 band gap

3.17
dislocation
linear crystallographic defect in monocrystalline material

[SOURCE: IEC 63068-1:2019, 3.22]

3.18
Burgers vector
vector representing the magnitude and direction of lattice distortion along a dislocation in monocrystalline material, which is denoted by ***b*** in this document

[SOURCE: IEC 63068-1:2019, 3.42, modified – The explanation "which is denoted by ***b*** in this document" has been added.]

3.19
edge dislocation
dislocation whose Burgers vector is perpendicular to the dislocation line

3.20
screw dislocation
dislocation whose Burgers vector is parallel to the dislocation line

3.21
threading dislocation
dislocation penetrating through the crystal approximately normal to the basal plane

3.22
transmission electron microscopy
TEM
technique employed to observe defect structures and wafer crystalline using a high voltage electron beam-penetration

3.23
optical microscopy
OM
technique employed to observe morphological features of wafer surface through the magnification by lenses with visible light

[SOURCE: IEC 63068-1:2019, 3.45]

3.24
macroscopic dislocation
dislocation which can be observed by naked eye directly

4 Classification of defects

4.1 General

The classification of defects in GaN epitaxial film on 4H-SiC (0001) and 6H-SiC (0001) substrate in this document is based on crystallographic type and dimension of the defects. Defects in GaN epitaxial film on SiC substrate shall be categorised into 11 patterns as given in Table 1.

Table 1 – Classification of defects in GaN epitaxial film on SiC substrate

No.	Type of defect	Dimension of defects	Figure
1	Vacancy	Point	Figure 1
2	Interstitial		Figure 2
3	Substitutional defect		Figure 3
4	Point defect complex		Figure 4
5	Threading dislocation	Linear	Figure 5
6	Crack	Volume	Figure 6
7	Inclusion		Figure 7
8	Hillock	Surface defects	Figure 8
9	Pit		Figure 9
10	Scratch		Figure 10
11	Others	Not specified	None

4.2 Description of the defect classes

4.2.1 General

The terminologies and schematic illustrations of each defect are shown in 4.2.2 to 4.2.11. Schematic illustrations, optical microscope images, or transmission electron microscope images are given based on the characteristics of each defect, respectively.

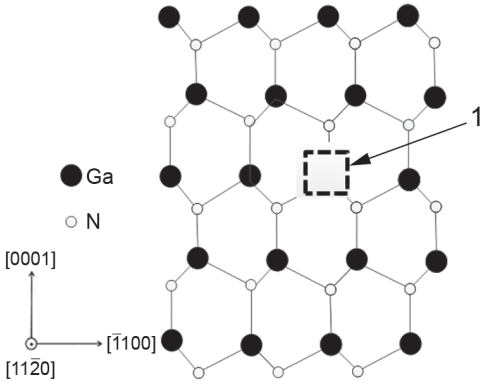
4.2.2 Vacancy

Vacancy space caused by the atom in the lattice site leaving its lattice site is called vacancy.

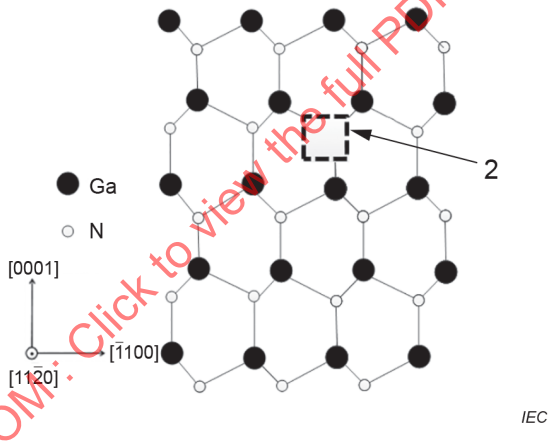
NOTE 1 Vacancy formed by an atom leaving its lattice site and escaping to the surface of the crystal is called Schottky defect and the defect is alone inside the crystal.

NOTE 2 Vacancy formed by an atom displacing from its lattice site to an interstitial site is called Frenkel defect and the defect is coupled with an interstitial atom.

NOTE 3 In GaN epitaxial film, the vacancy could be classified into two categories: gallium vacancy (V_{Ga}), caused by the absence of a gallium atom, as shown in Figure 1 a); nitrogen vacancy (V_N), caused by the absence of a nitrogen atom, as shown in Figure 1 b).



a) Schematic illustration of V_{Ga}



b) Schematic illustration of V_N

Key

1 V_{Ga}

2 V_N

Figure 1 – Vacancy

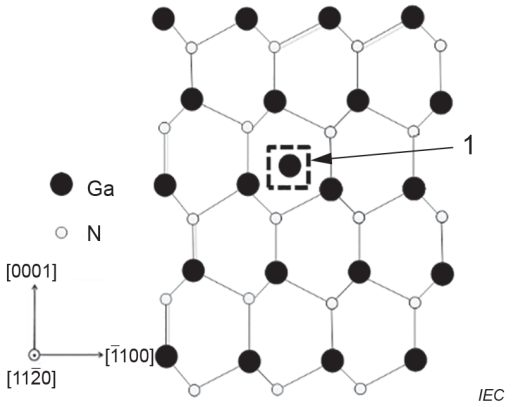
4.2.3 Interstitial

Additional atom existing at the interstitial site of a crystal is called interstitial.

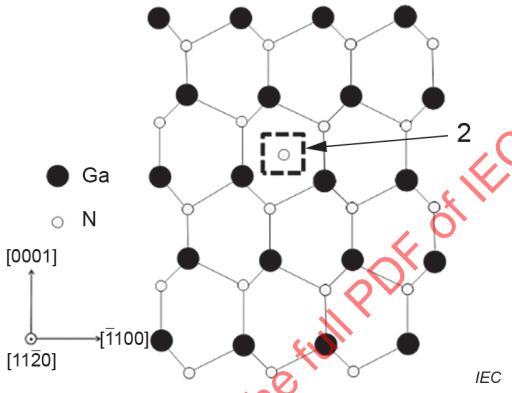
NOTE 1 In GaN epitaxial film, the interstitial can be classified into two categories: self-interstitial or impurity interstitial.

NOTE 2 Self-interstitial is additional gallium or nitrogen atoms at the interstitial site of the crystal. Figure 2 a) and Figure 2 b) show a gallium interstitial (Ga_i) and a nitrogen interstitial (N_i), respectively.

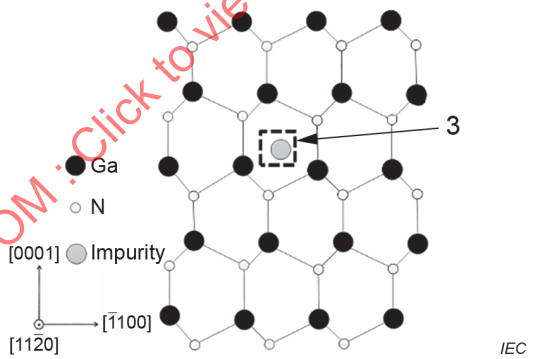
NOTE 3 Impurity interstitial (I_i) is formed when the impurity atom is packed into the interstitial site of the crystal, as shown in Figure 2 c).



a) Schematic illustration of Ga_i



b) Schematic illustration of N_i



c) Schematic illustration of I_i

Key

1 Ga_i

2 N_i

3 I_i

Figure 2 – Interstitial

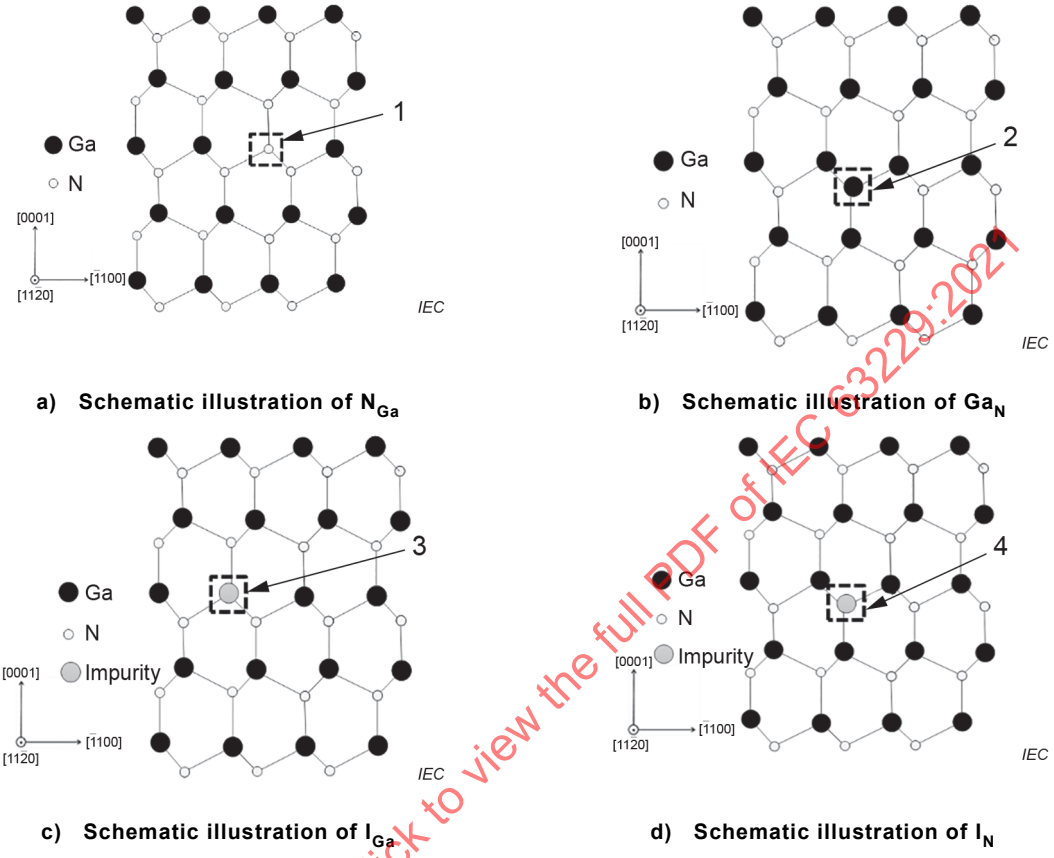
4.2.4 Substitutional defect

The lattice site occupied by an atom that does not originally exist at the site are called substitutional defects.

NOTE 1 Substitutional defect could be classified into two categories: anti-site substitutional defect and impurity substitutional defect.

NOTE 2 Anti-site substitutional defect could be formed when the lattice site of the Ga is replaced by an N atom (N_{Ga}), or the lattice site of the N is replaced by a Ga atom (Ga_N). Figure 3 a) and Figure 3 b) show the schematic illustrations of N_{Ga} and Ga_N anti-site substitutions, respectively.

NOTE 3 Impurity substitutional defect could be formed when the lattice atom is replaced by the impurity atom. Figure 3 c) and d) show the impurity substitutional defect of lattice site of the Ga (I_{Ga}) and lattice site of the N (I_N), respectively.



a) Schematic illustration of N_{Ga}

b) Schematic illustration of Ga_N

c) Schematic illustration of I_{Ga}

d) Schematic illustration of I_N

Key

1 N_{Ga}
2 Ga_N
3 I_{Ga}
4 I_N

Figure 3 – Substitutional defect

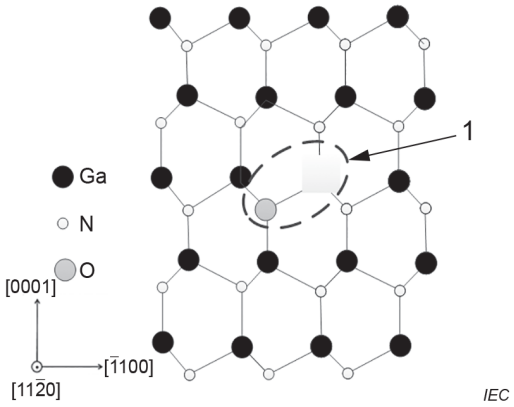
4.2.5 Point defect complex

Two or more point defects interacting with each other and forming complex are called point defect complex.

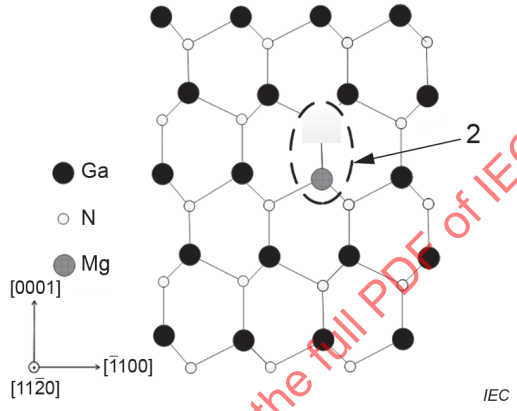
NOTE 1 Point defect complex in the GaN epitaxial film is generally divided into shallow donor gallium vacancy complex and shallow acceptor nitrogen vacancy complex.

NOTE 2 Shallow donor gallium vacancy complex is point defect complex composed of gallium vacancy and other point defects, such as V_{Ga}-O_N [Figure 4a)] and V_{Ga}-Si_{Ga}, in which O_N refers to the lattice site of N replaced by an O atom, Si_{Ga} refers to the lattice site of Ga replaced by a Si atom.

NOTE 3 Shallow acceptor nitrogen vacancy complex means point defect complex composed of nitrogen vacancy and other point defects, such as Mg_{Ga}-V_N [Figure 4b)] and Si_{Ga}-V_N, in which Mg_{Ga} refers to the lattice site of Ga replaced by a Mg atom, Si_{Ga} refers to the lattice site of Ga replaced by a Si atom.



a) Schematic illustration of point defect complex of V_{Ga}-O_N



b) Schematic illustration of point V defect complex of Mg_{Ga}-V_N

Key

1 Point defect complex of V_{Ga}-O_N

2 Point defect complex of Mg_{Ga}-V_N

Figure 4 – Point defect complex

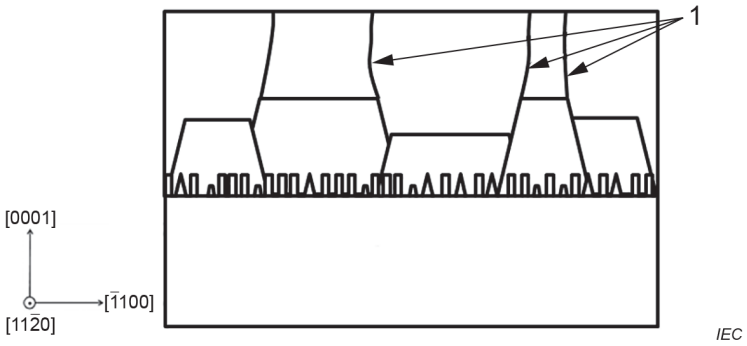
4.2.6 Threading dislocation

Dislocation that propagates through the GaN epitaxial film, is called threading dislocation, as shown in Figure 5 a).

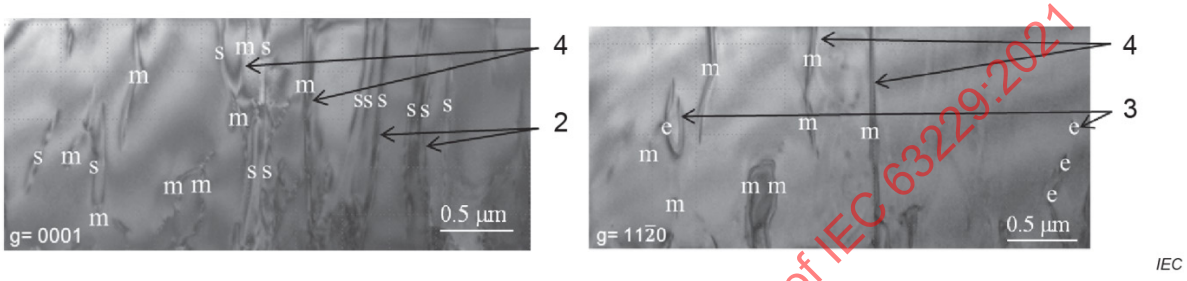
NOTE 1 There are three types of threading dislocation in GaN epitaxial film grown along the c-axis [0001]: pure edge dislocation with the Burgers vector ***b*** = 1/3 <11$\bar{2}$0>; pure screw dislocation with Burgers vector ***b*** = <0001>; mixed dislocation with Burgers vector ***b*** = 1/3<11$\bar{2}$3>.

NOTE 2 Figure 5 b) shows TEM images of threading dislocation in GaN epitaxial layer grown on SiC substrate.

NOTE 3 Figure 5 b) shows TEM images collected using a TEM equipment operating at 200 kV acceleration energy under g = 0001 and 11$\bar{2}$0 diffraction conditions.



a) Schematic illustration of threading dislocation



b) TEM images of edge dislocation (e), screw dislocation (s) and mixed dislocation (m)

Key

1 Threading dislocation

2 Screw dislocation

3 Edge dislocation

4 Mixed dislocation

Figure 5 – Threading dislocation

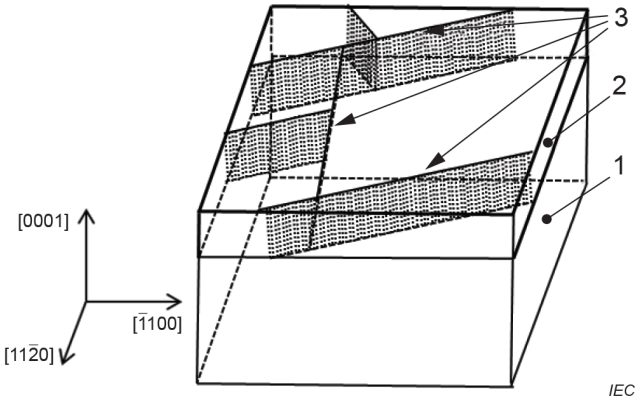
4.2.7 Crack

A fracture caused by stress propagating from the epitaxial interior to the surface is called crack, as shown in Figure 6 a).

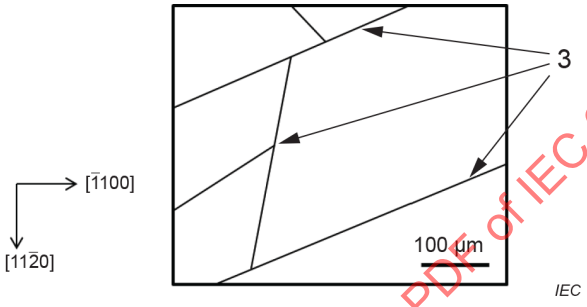
NOTE 1 A crack is a macroscopic dislocation propagating from the epitaxial interface to the surface and is usually straight and can cross other cracks.

NOTE 2 Figure 6 b) and Figure 6 c) show plan-view observation image and OM image of crack in GaN epitaxial layer grown on SiC substrate, respectively.

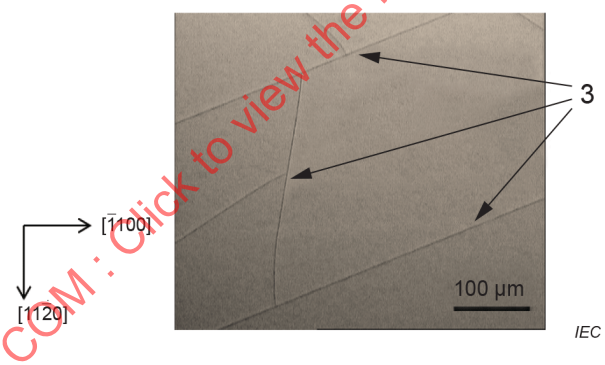
NOTE 3 Figure 6 c) was collected using an OM equipment with light source operating at 10 V and 5 A under bright-field.



a) Schematic illustration of crack



b) Plan-view observation image of crack



c) OM image of crack

Key

1 SiC substrate

2 GaN epitaxial layer

3 Crack

Figure 6 – Crack

4.2.8 Inclusion

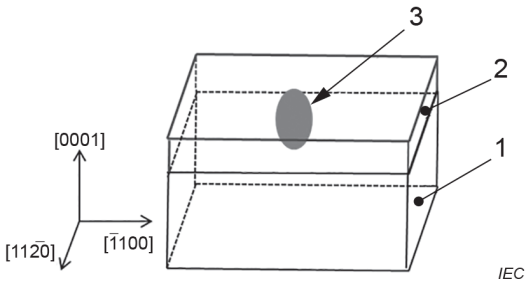
Particle or impurity enveloped in the GaN epitaxial layer is called inclusion, as shown in Figure 7 a).

NOTE 1 Inclusion is caused by particle falling on the substrate surface before, or during epitaxial growth.

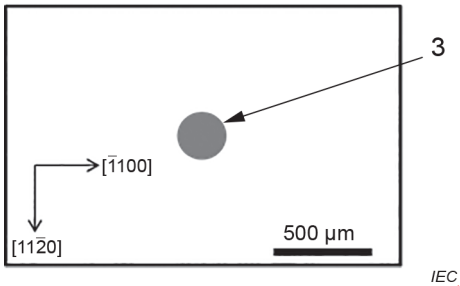
NOTE 2 Inclusion can not only lie in epitaxial layer, but can also be observed on the epitaxial film surface.

NOTE 3 Figure 7 b) and c) show plan-view observation image and OM image of inclusion in GaN epitaxial layer grown on SiC substrate, respectively.

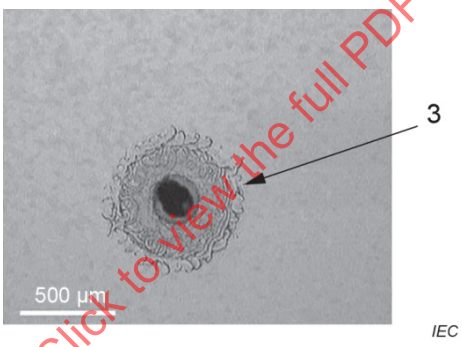
NOTE 4 Figure 7c) shows an inclusion collected using an OM equipment with light source operating at 10 V and 5 A under bright-field.



a) Schematic illustration of inclusion



b) Plan-view observation image of inclusion



c) OM image of inclusion

Key

1 SiC substrate

2 GaN epitaxial layer

3 Inclusion

Figure 7 – Inclusion

4.2.9 Hillock

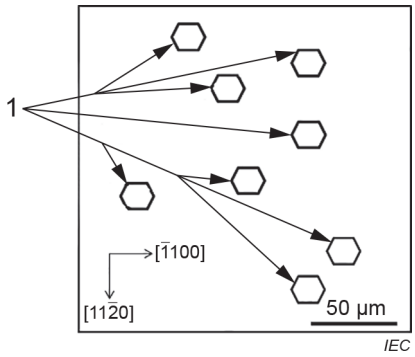
The convex structure at the surface of the epitaxial film is called hillock.

NOTE 1 During the epitaxial growth process, a tiny region would grow faster than its surroundings if the growth conditions are irrelevant, or some drops lead to formation of a hillock. At the onset of growth, the large flux of ammonia is conducive to the surface formation of hexagonal hillock structures.

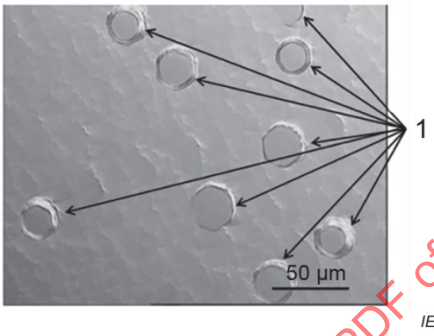
NOTE 2 The possible shapes of hillock include: hexagonal trapezoidal, pyramidal, and others.

NOTE 3 Figure 8 a), Figure 8 c), and Figure 8 e) show plan-view observation image of hexagonal trapezoidal hillock, incomplete hexagonal trapezoidal hillock and pyramidal hillock in the GaN epitaxial layer grown on SiC substrate, respectively. And Figure 8 b), Figure 8 d), and Figure 8 f) show OM images corresponding to Figure 8 a), Figure 8 c), and Figure 8 e).

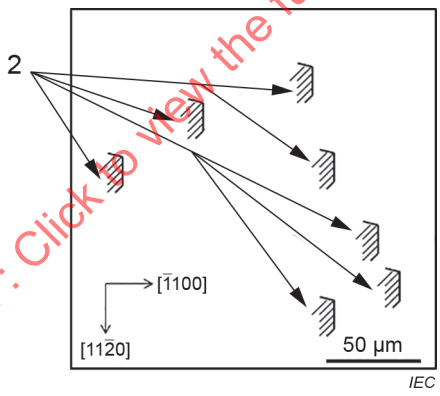
NOTE 4 Figure 8 b), Figure 8 d), and Figure 8 f) show images collected using an OM equipment with light source operating at 10 V and 5 A under bright-field.



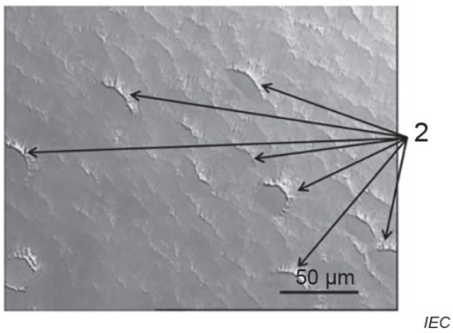
a) Plan-view observation image of hexagonal trapezoidal hillock



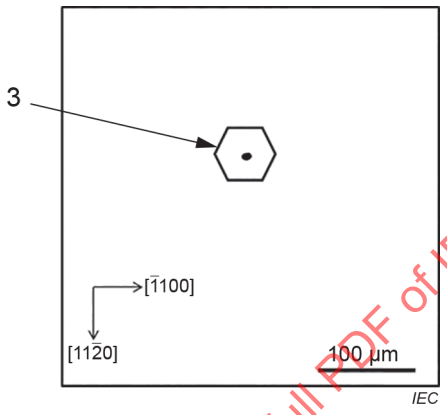
b) OM image of hexagonal trapezoidal hillock



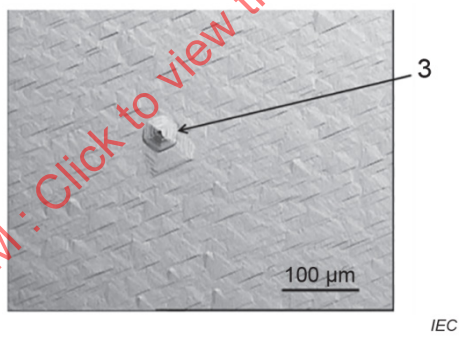
c) Plan-view observation image of incomplete hexagonal trapezoidal hillock



d) OM image of incomplete hexagonal trapezoidal hillock



e) Plan-view observation image of pyramidal hillock



f) OM image of pyramidal hillock

Key

1 Hexagonal trapezoidal hillock

2 Incomplete hexagonal trapezoidal hillock

3 Pyramidal hillock

Figure 8 – Hillock

4.2.10 Pit

Hollow at the surface of the epitaxial film is called pit.

NOTE 1 A region of growth terminated by unsuitable growth conditions or drop, leading to pitting at the film surface.

NOTE 2 Figure 9 a) and Figure 9 b) show plan-view observation image and OM image of pit caused by drop in GaN epitaxial film grown on SiC substrate.

NOTE 3 Figure 9 c) and Figure 9 d) show plan-view observation image and OM image of hexagonal pit in GaN epitaxial film grown on SiC substrate.