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The structure and optoelectronic properties of dislocations in GaN

D Cherns
HH Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK

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Abstract. This paper reviews the structure of threading dislocations, nanopipes and inversion domains in (0001) GaN films grown by metal–organic chemical vapour deposition. A new mechanism for generation of misfit dislocations in epitaxial laterally overgrown (ELOG) GaN and in AlGaN/GaN interfaces is described. Recent cathodoluminescence studies in the scanning electron microscope are described, showing that individual threading defects act as non-radiative recombination centres in ELOG GaN and in InGaN quantum wells in GaN.

1. Introduction

In the last few years, GaN/InGaN/AlGaN structures have become the basis of new commercial light-emitting diodes and lasers working at the blue end of the visible spectrum. Yet these developments are particularly surprising given that most devices have densities of threading defects exceeding 10^9–10^{10} cm^{-2}. In contrast light-emitting devices based on GaAs fail at defect densities greater than 10^4–10^5 cm^{-2} [1]. There is, thus, great interest in understanding why threading defects in GaN structures are, apparently, so benign. To examine this problem, we have investigated the structure of a variety of threading defects in GaN single layers and heterostructures by transmission electron microscopy (TEM) and the optical properties of individual defects using cathodoluminescence in the scanning electron microscope (SEM-CL). This paper reviews some recent results.

The materials described here were grown by metal–organic chemical vapour deposition (MOCVD), mainly on (0001) sapphire substrates. Under these conditions the GaN layers grow in the hexagonal wurtzite structure in (0001) orientation with a (predominantly) [0001] growth direction, i.e. with a 'Ga growth surface'. Section 2 describes some of the threading defects observed, namely dislocations, nanopipes and inversion domains, although, as most of this work has been published previously, only a brief summary is given. The generation of misfit dislocations in heterostructures is considered in section 3. This is of particular significance in GaN devices. Firstly, there is no simple relaxation mechanism, such that layer strains are often much larger than expected on equilibrium grounds. Secondly, these layer strains lead to large piezoelectric fields, which have dramatic effects on device properties (such as the quantum confined Stark effect—a red shift in luminescence [2], and increased carrier recombination times [3]). Recent studies of strain relaxation in epitaxial laterally overgrown (ELOG) GaN are illustrated. These demonstrate that strain relaxation occurs on the basal (0001) plane where shear stresses are present. It is shown that misfit dislocations can be generated by a similar mechanism in AlGaN/GaN films; the nature of the new mechanism which involves both glide and climb is discussed.

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Section 4 describes recent SEM-CL studies of individual threading defects in GaN and InGaN/GaN films. It is shown that threading defects in an ELOG GaN film act as non-radiative recombination centres. The effect of individual threading defects on the quantum well samples is also examined. It is shown that defects linked to screw dislocations act as 'black holes' in the QW emission although the net effect on luminescence is excitation dependent.

2. Threading defects in GaN epilayers

(0001) GaN thin films contain a variety of threading defects. We have examined the structure of dislocations, nanopipes and inversion domains (see [4] for a review). Dislocations in (0001) GaN films belong to all three main types common in hexagonal structures, namely those of $\boldsymbol{a}$ type (Burgers vector $\boldsymbol{b} = \frac{1}{3}\langle 11\bar{2}0\rangle$, $\boldsymbol{c}$ type ($\boldsymbol{b} = \langle 0001\rangle$) and $\boldsymbol{c}+\boldsymbol{a}$ type ($\boldsymbol{b} = \frac{1}{3}\langle 11\bar{2}3\rangle$) [5]. Weak beam studies of threading segments, which lie close to the c-axis, show no evidence of dissociation, although there is good evidence that basal plane segments dissociate into partials [6]. A distinctive feature of some GaN films in the presence of nanopipes. These are hollow tubes with diameters 5–30 nm and $\{10\bar{1}0\}$ facetted sides. We have shown by large angle convergent beam electron diffraction (LACBED) that some nanopipes are hollow core screw dislocations with Burgers vectors $\boldsymbol{b} = \pm\boldsymbol{c}$ [7].

The question of whether nanopipes are an equilibrium form of screw dislocations has been considered by a number of groups. Frank [8] first proposed that dislocations might generate a hollow core to lower total energy, by relieving strain energy at the expense of free surface energy. Frank gave the equilibrium radius r as

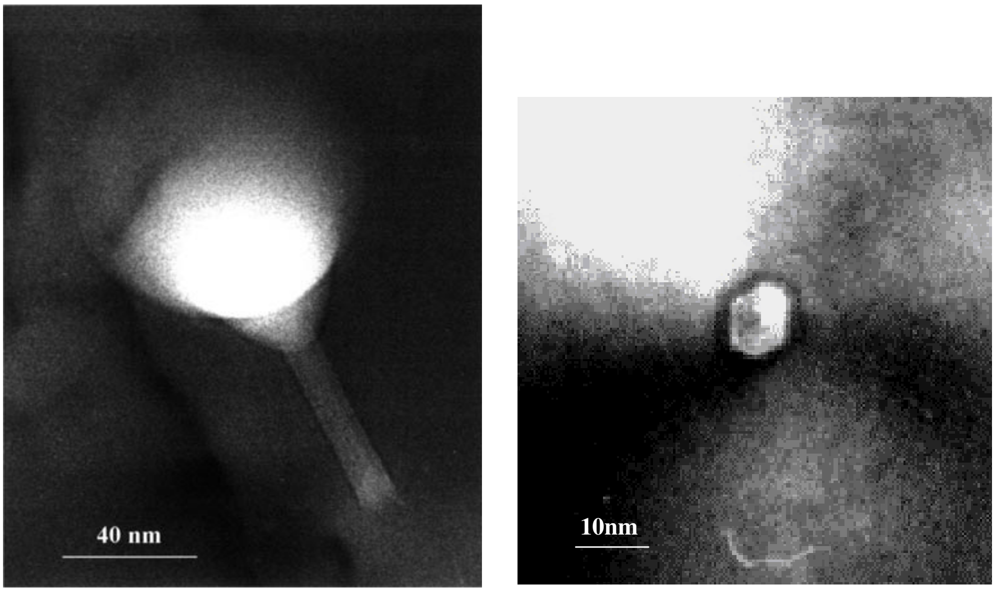
$$r = \mu b^2/8\pi^2\gamma \tag{1}$$

where μ is the shear modulus and γ is the surface energy. Calculations for nanopipes in GaN suggest that $r \sim$ atomic dimensions ($b = 0.52$ nm), much smaller than the experimental value. It is thus likely that nanopipes form under non-equilibrium conditions and that local growth factors are important. We have suggested that nanopipes may grow from pinholes present during the early stages of growth [7]. More recently we have studied nanopipes in GaN samples which were heavily Si doped (10^{19} cm^{-3}). In these samples some nanopipes had either constrictions over part of their length or opened out into larger pits. Figure 1 shows two examples. In the top picture, a nanopipe viewed obliquely has expanded into a micron-sized cone. In the bottom picture, a nanopipe viewed end-on is constricted such that an undissociated screw dislocation is formed; the contrast from the end-on dislocation can be clearly seen.

A more extensive study of the sample in figure 1 showed that there was no correlation between the changes in nanopipe diameter and depth in the foil, with adjacent screw dislocations showing quite different behaviour. Given the general observation that MOCVD-grown GaN has stable growth on both the $\{10\bar{1}0\}$ and $\{10\bar{1}1\}$ facets, this implies that growth transitions were important and were statistical in nature, i.e. growth accidents. It is, thus, tempting to suppose that these growth transitions were initiated by the Si doping. It is worth noting that observations on a range of samples have shown that densities of nanopipes are indeed affected by a range of dopants including Si (see [9] for a review). However, more work is clearly needed to establish the specific role (if any) of the Si and the atomic level mechanism involved.

3. Accommodation of misfit strains in GaN and AlGaN/GaN films

GaN/InGaN/AlGaN structures can have large lattice mismatches since the basal plane lattice spacings of InN and AlN are respectively 10% greater and 3% smaller than that of GaN.



(a) (b)

Figure 1. TEM images of nanopipes in a plan-view MOCVD-grown GaN sample heavily doped with Si (10^{19} cm^{-3}): (a) a nanopipe opening out to form a micron-sized cone, (b) a nanopipe viewed end-on which has constricted over part of its length to give an undissociated screw dislocation, seen by its characteristic black–white contrast. (Courtesy of H Mokhtari).

We might expect lattice relaxation to occur quite readily given that $\boldsymbol{a}$ and $\boldsymbol{c}+\boldsymbol{a}$ dislocations could act as misfit dislocations and high densities of these dislocations are generally present. In practice these dislocations do not often act as misfit dislocations. We may contrast this behaviour with that in cubic (001) semiconductor heterostructures where threading dislocations act as misfit dislocation sources by the Matthews and Blakeslee mechanism (see [10] for a review). This involves dislocation glide on inclined {111} planes in response to shear stresses. Jesser and Matthews [11] gave the critical resolved shear stress as

$$\tau = 2\mu\varepsilon[(1+\nu)/(1-\nu)]\cos\phi\cos\lambda \tag{2}$$

where ϕ is the angle between the film surface and the normal to the slip plane, λ is the angle between the slip direction and the direction in the interfacial plane perpendicular to the line of intersection of the slip plane and the interface, ν and ε are Poisson's ratio and the in-plane strain respectively. The same mechanism does not operate in (0001) GaN heterostructures since inclined slip planes, such as $\{10\bar{1}1\}$, are not generally active. Slip on the basal plane is possible but has $\phi = 90^\circ$ and hence $\tau = 0$.

In recent work we have examined misfit strain relief in epitaxial laterally overgrown (ELOG) GaN films [12]. Figure 2 shows an overgrown region in a plan-view specimen. The seed crystal on the right-hand side, which has grown through a gap between SiO_2 strips running in a $\langle 10\bar{1}0\rangle$ direction, has an array of threading dislocations. Boundaries between the ELOG material and the seed crystal, and an adjoining overgrown region on the left-hand side, contain long in-plane dislocations which accommodate small crystal rotations (less than 1°) along both vertical and horizontal axes lying in the basal plane. The two curved dislocations in the ELOG region are of $\boldsymbol{a}$ type, and contain basal plane segments which terminate in a threading segment. The threading segment for one of these dislocations can be seen. It is

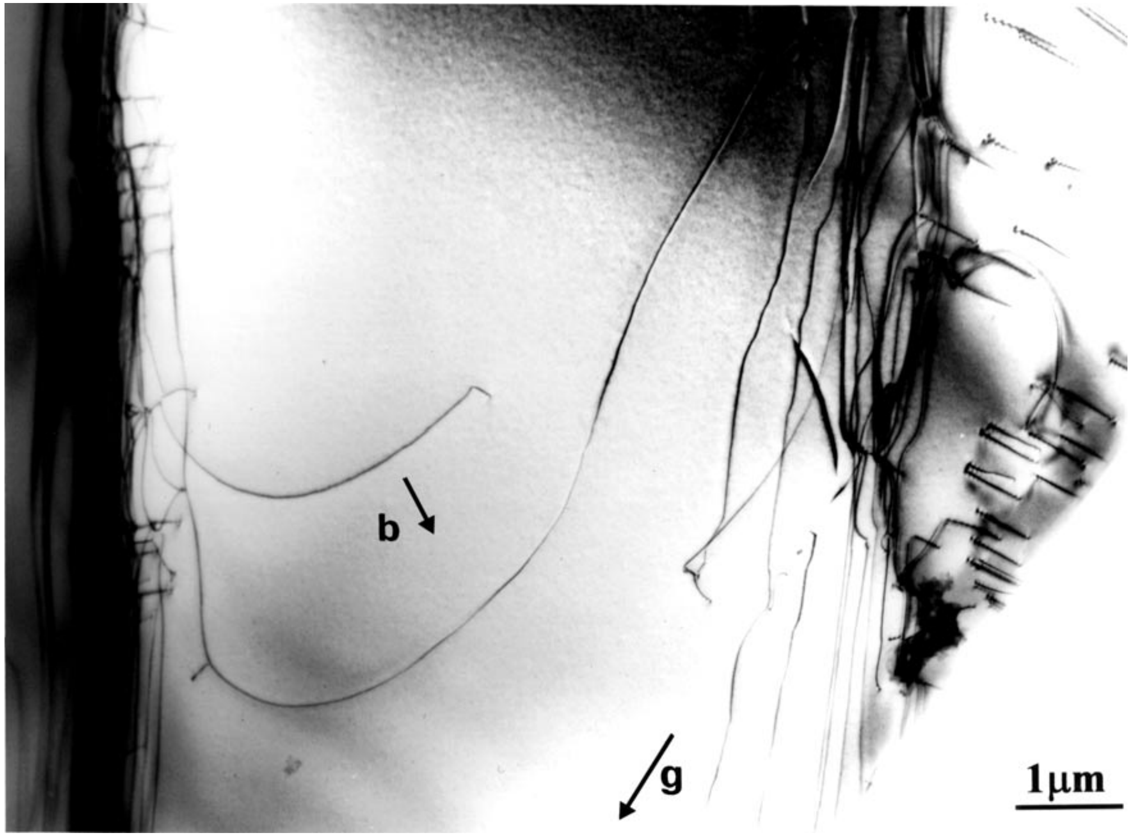


Figure 2. A plan-view sample of ELOG GaN which has been tilted to show threading dislocations in the seed crystal (right-hand side) obliquely inclined, the boundary between the seed crystal and the laterally overgrown material (right) and the boundary between laterally overgrown crystals (left). The image is taken under two-beam diffracting conditions with $g = \langle 11\bar{2}0\rangle$. The two $\boldsymbol{a}$-type dislocations in the mainly defect free central region (Burgers vector shown) are believed to have propagated under shear stresses generated during cooling immediately after film growth. (Courtesy of Z Liliental-Weber).

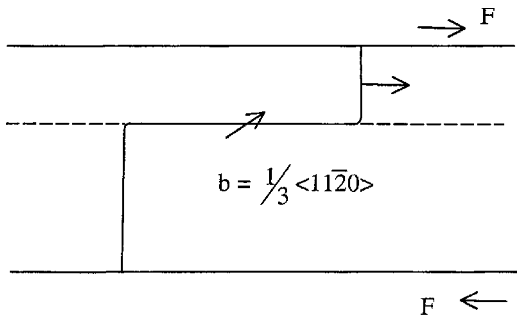


Figure 3. Proposed dissociation of a threading $\boldsymbol{a}$-type dislocation under the action of a shear stress F acting on the basal plane. To operate, a combination of glide in the basal plane and climb of the threading segment is required.

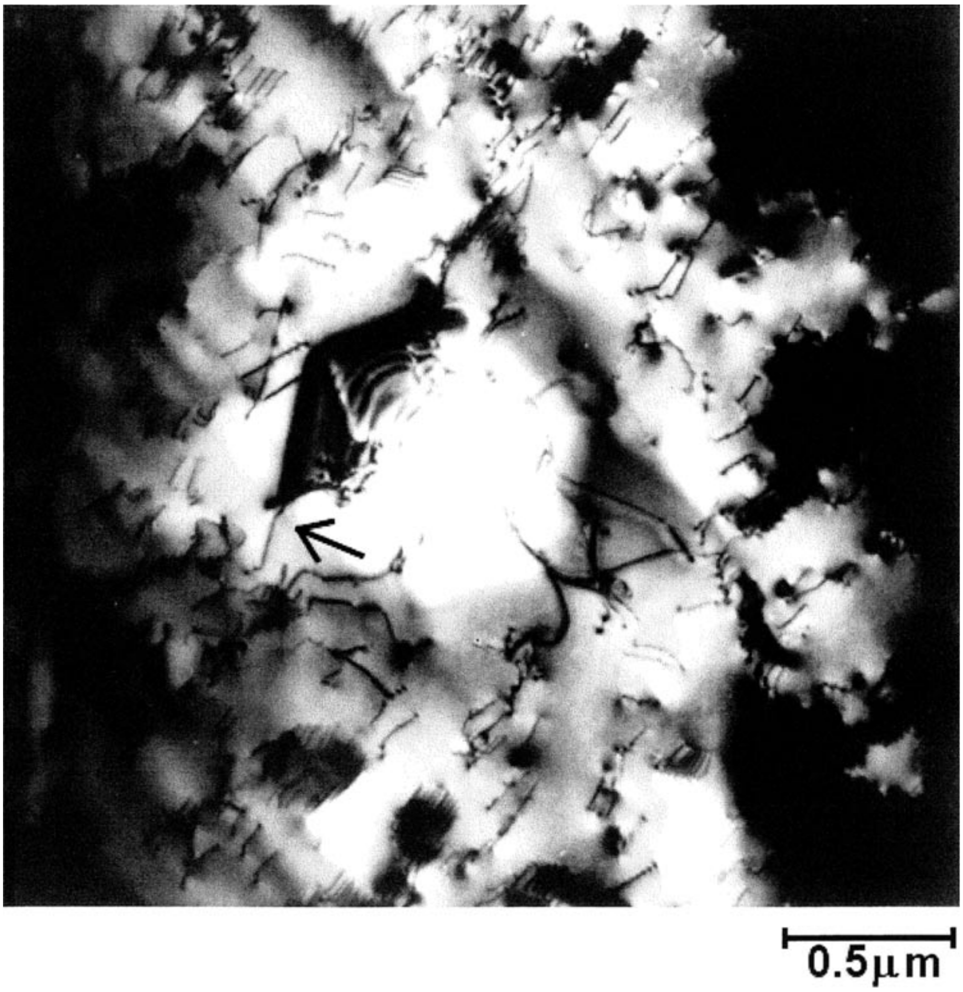
believed that these dislocations originate from the dissociation of a threading dislocation by the mechanism illustrated in figure 3. We believe that the driving force for this mechanism is a shear stress generated on the basal plane along the stripe direction during cooling from the growth temperature due to the thermal mismatch between SiO_2 and GaN (see [12] for more details). The mechanism involves glide on the basal plane, although the end threading segment, which is not in the slip plane, must clearly move by climb.

We have observed the generation of misfit dislocations in AlGaN/GaN films by a closely similar mechanism [13]. Figure 4 shows several misfit dislocations emanating from a V-shaped pit. The foil has been tilted by several degrees off the [0001] axis such that threading dislocations lying close to the c-axis are seen in projection. Around the pit there are also dislocations which are clearly aligned in different directions. These have in-plane segments terminating in a threading segment. An example is seen in the blown-up region, the threading segment sharing oscillatory contrast indicating the changing depth in the foil.

A more extensive analysis showed that dislocations of the type seen in the blown-up region were threading dislocations which originated within the pitted region, and that the in-plane segments which extended outside the pitted region were close to the AlGaN/GaN interface. A Burgers vector analysis also indicated that these dislocations were predominantly of $\boldsymbol{a}$ type with in-plane components having orientations generally close to edge type. We can thus infer that the dissociation process is similar to that seen in figure 3 and that the generation process involves both glide and climb. It is interesting that outside the pit, the shear stress is zero (ignoring some foil bending) confirming that the process is essentially driven by the climb force. It is believed, however, that the process is initiated by shear stresses that act on the basal plane where the AlGaN/GaN interface is inclined (on the $\{10\bar{1}1\}$ pit facets). The presence of these shear stresses causes a slight rotation of the $\{11\bar{2}0\}$ diffracting planes in figure 4 explaining the strong diffraction contrast seen around the pit edges. The fact that dislocations well separated from the pit have, generally, not dissociated to form misfit dislocations suggests that there exists an energy barrier to the initial dissociation.

4. Cathodoluminescence studies of threading defects

The effect of threading dislocations and other defects on GaN light-emitting devices is still not resolved. CL studies have shown that some defects, at least, in GaN films act as non-radiative recombination centres, but that the carrier migration distance is small, ranging from about 0.25 μm [14] to much lower values depending on doping (e.g. see [15]). We have studied CL



(a)

(b)

Figure 4. Threading dislocations intersecting a V-shaped pit in AlGaN/GaN are believed to dissociate initially by the mechanism in figure 3, under shear stresses generated on the pit facets where the AlGaN/GaN interface is inclined. (Courtesy of O Evans).

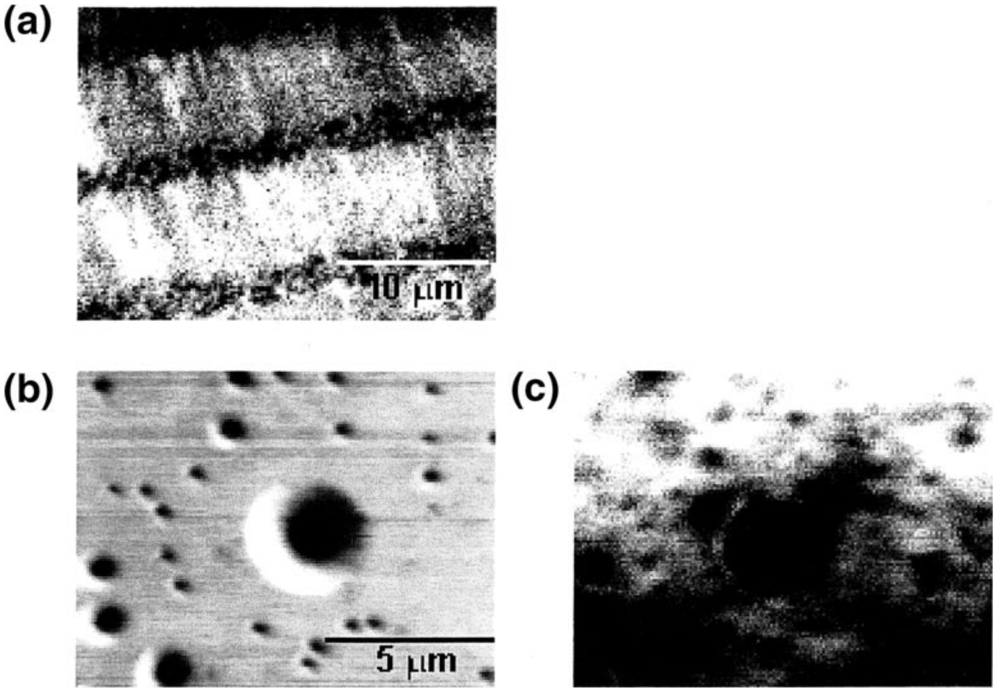


Figure 5. (a) CL image in the band edge luminescence (356 nm) from an ELOG GaN film showing reduced luminescence in bands running along a $\langle 10\bar{1}0\rangle$ axis corresponding to the seed crystal where threading dislocations are present, (b) and (c) show respectively a secondary electron image and an image at 460 nm from a GaN/InGaN/GaN sample. (Courtesy of S J Henley).

at temperatures down to $\sim$8 K in a modified field emission gun SEM, as described previously [16]. Figure 5(a) shows a CL map in the band edge emission from an ELOG GaN sample. The dark spots can be tentatively ascribed to threading dislocations in the seed regions, although a direct correlation has not yet been done. The much brighter CL in the overgrown regions show some striations in the contrast; it may be that this is due to some relaxation of the type seen in figure 2.

In recent work we have examined the effect of threading defects on the quantum well (QW) luminescence from InGaN/GaN structures. Figure 5(b) and (c) show an example from a single quantum well structure containing a 1.5 nm $In_{0.28}Ga_{0.72}N$ QW buried with a 30 nm GaN capping layer [17]. The CL image was recorded at low voltage (5 kV) to restrict the beam penetration to the region adjacent to the QW and thus maximize the QW luminescence. The QW luminescence is seen to be quenched in regions which correspond to a series of large and small pits, which are clearly visible in the secondary electron image (figure 5(b)).

TEM studies showed that the pits in figures 5(b) and (c) were mostly associated with threading defects including nanopipes. However the absence of QW luminescence can be simply attributed to the fact that the InGaN QW was absent from the pit facets rather than an intrinsic property of the defects themselves. Between the pits there is also a high density of threading dislocations, predominantly with $\boldsymbol{a}$-type Burgers vectors. Whether these defects act as non-radiative centres in the QW emission has, however, not yet been resolved.

Line profiles across images of the type in figure 5(c) showed that the effective carrier diffusion length was both small and dependent on the excitation conditions, increasing from less than 0.2 to 0.33 μm upon continued irradiation [17]. This effect, which was accompanied by a blue shift in the QW emission has been attributed to the filling of trap states in the QW, possibly due to In fluctuations, and a screening of the strain-induced piezoelectric field. The inference is that the net influence of individual threading defects on luminescence of devices is dependent partly on the operating conditions.

Acknowledgments

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