PHYSICAL REVIEW B VOLUME 60, NUMBER 12 15 SEPTEMBER 1999-II

Indium-induced changes in GaN(0001) surface morphology

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(Received 1 June 1999; revised manuscript received 16 July 1999)

First-principles calculations of the energetics of the In-terminated GaN(0001), (000$\underline{1}$), (10$\underline{1}$1), and (10$\underline{11}$) surfaces indicate that In has a substantial effect on the relative energies of formation of these surfaces. Indium-induced changes in the surface energetics enable the formation of inverted hexagonal pyramid defects having (10$\underline{1}$1) facets at the termination of threading defects on the (0001) surface of pseudomorphic $In_xGa_{1-x}N$ films. For dislocations terminating on the $In_xGa_{1-x}N$(000$\underline{1}$) surface, the calculations predict that large (10$\underline{11}$) faceted defects are not energetically favorable. [S0163-1829(99)52036-5]

There is currently a high degree of interest in understanding the diverse mechanisms which determine the growth morphology of epitaxial films.[1] This interest is almost invariably driven by a technological application. The use of $In_xGa_{1-x}N$ quantum wells to form the active region of blue lasers and light emitting diodes has generated much interest in issues related to their growth.[2] Investigations have revealed many interesting features of epitaxial $In_xGa_{1-x}N$ films including compositional fluctuations,[3] chemical ordering,[4] surfactant behavior,[5] and the formation of a unique defect, the inverted hexagonal pyramid defect.[6–10] To understand and eventually gain control over these phenomena, which directly affect the optoelectronic properties of the material, it is essential to know how In interacts with the surface of the growing film. In this article we present theoretical studies to determine the behavior of In on GaN surfaces.

The term surfactant is used often to denote a substance that modifies the growth morphology of an epitaxial film, either by changing the surface energy or altering adatom mobility. In some cases it may be useful to employ a more specific definition—differential surfactant—to denote an element that substantially changes the *relative* energies of two surface orientations of a material to such an extent that the morphological evolution of an epitaxial film is altered during growth. We show here that In is such a differential surfactant on GaN. Under the N-rich conditions required for their incorporation, the In atoms have a large effect on the relative energies of the (0001) and the (10$\underline{1}$1) surfaces of GaN. This leads to a dramatic change in the growth morphology of $In_xGa_{1-x}N$ alloys through the formation of (10$\underline{1}$1) faceted dislocation pits at the termination of threading dislocations on the (0001) surface.

The termination of a threading dislocation at the surface of a growing film may in some cases lead to the formation of a pit on the surface of the film. The energetic driving force to form a pit is the reduction in energy achieved by avoiding the accumulation of strained material in the region near the core of the dislocation. This reduction in strain energy is accomplished at the expense of increased surface energy, and the size and shape of the pit is affected by the surface and dislocation energetics.[11,12] For pseudomorphic $In_xGa_{1-x}N$ films grown on GaN(0001), the termination of the dislocation gives rise to a specific type of pit known alternatively as an inverted hexagonal pyramid (IHP), a hexagonal pinhole, or as a *V* defect.[6–10] In forming an IHP, a hexagonal region of the (0001) surface is replaced with six (10$\underline{1}$1) sidewall facets, as indicated schematically in Fig. 1. We recently reported structural models and energetics for the (10$\underline{1}$1) surface and conjectured that In termination would reduce the surface energies sufficiently to enable the formation of large IHP defects.[12] This paper provides justification for this proposal. In addition, we show that in contrast to the behavior expected for growth on the $In_xGa_{1-x}N$(0001) surface, formation of large IHP defects is *not* expected for growth on the $In_xGa_{1-x}N$(000$\underline{1}$) surface.

This paper intends to demonstrate that the energy reduction arising from surface termination by In rather than Ga is much greater for the (10$\underline{1}$1) surface in comparison to the (0001) surface. The difference is a consequence of the different binding sites available for In on the two surfaces. On the (0001) surface, the In incorporates in adlayer sites and in threefold coordinated sites, in which it forms bonds to three N atoms. On the (10$\underline{1}$1) surface, it binds in sites where it makes one or two bonds with the N atoms in the subsurface layer. We refer to the adlayer site as an $A1$ site, the threefold site as an $S3$ site, the onefold as a $T1$ site, and the twofold sites as a $B2$ site. The surfaces and the binding sites are indicated schematically in Fig. 2. Our calculations indicate that the energy reduction achieved by substituting In for Ga atoms is much larger for the $A1$, $T1$, and $B2$ sites than for

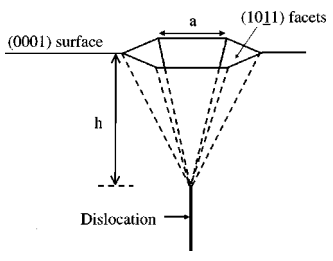

FIG. 1. Schematic representation of a dislocation terminating in a hexagonal pit at the (0001) surface. A hexagonal shaped pit of lateral size *a* and depth *h* forms to reduce the energy associated with the dislocation. Pit formation exposes the six equivalent (10$\underline{1}$1) facets.

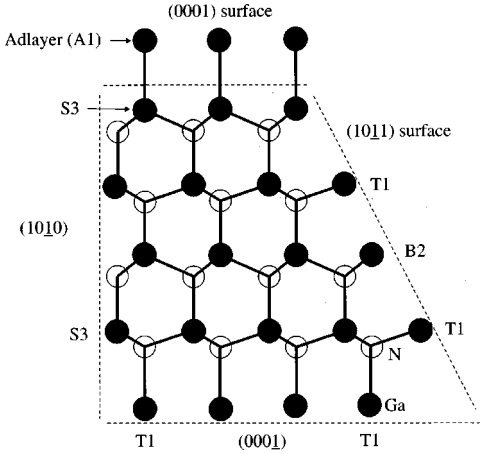

FIG. 2. Schematic representation of the (0001), (10$\underline{1}$1), (000$\underline{1}$), and (10$\underline{1}$0) surfaces. $S3$, $B2$, and $T1$ sites are those in which Ga or In forms 3, 2, or 1 bonds to a N atom. The $A1$ sites are adlayer sites on the (0001) surface where the In or Ga is bonded to the In or Ga in the $S3$ sites below.

the $S3$ site, and that the energy required to create (10$\underline{1}$1) surfaces at the expense of (0001) surfaces is substantially reduced by the presence of In. This effect increases the size of the inverted hexagonal pyramid defects at the termination of threading dislocations on (0001) surfaces of $In_xGa_{1-x}N$ films.

To calculate the formation energy of an IHP defect, one may employ a simple model.[11,12] Consider the change in energy resulting from the formation of an IHP of size a and depth h as depicted in Fig. 1. Formation of the IHP reduces the strain energy and core energy arising from the dislocation. In forming the pit, a hexagonal shaped region of the (0001) surface is eliminated and replaced by six (10$\underline{1}$1) sidewall facets. We take the energy of the dislocation to be that of a simple screw dislocation with a small open core of radius $r=\mu b^2/8\pi^2\gamma_0$.[11] In this expression, $\mathbf{b}=c[0001]$ is the Burgers vector of the dislocation, μ is the shear modulus, and γ_0 is the surface energy of the open core sidewalls. For simplicity, we take γ_0 to be the energy ($\sim$120 meV/Å^2) of the (10$\underline{1}$0) prismatic plane. As discussed elsewhere, r is approximately 0.2 nm.[13] We measure lengths in terms of r, and energies in terms of $\gamma_0 r^2$. The energy that is required to form a large inverted pyramid of size $x=a/r$ is

$$\Delta E(x)=\gamma_0 r^2\{Sx^2-Cx\ln x\},$$

where C is a geometrical factor equal to $2\pi h/a$ [$C=10.26$ for (10$\underline{1}$1) facets], and S is the projected difference in the surface energies of the (0001) and the (10$\underline{1}$1) surfaces:

$$S=(3\sqrt{3})/2[\,\gamma(10\underline{1}1)/\alpha-\gamma(0001)]/\gamma_0$$

The factor $\alpha=\cos\theta=0.468$ appears in this expression because the (10$\underline{1}$1) surface makes an angle $\theta=62.1$ degrees with respect to the (0001) surface as shown in Fig. 1. The equilibrium size of the inverted hexagonal pyramid is determined by minimizing $\Delta E(x)$. Because the value of x that minimizes ΔE is independent of r, the equilibrium pit size is proportional to $\mu b^2/\gamma_0$. The critical parameter that controls the equilibrium size is the surface energy anisotropy S. It has been suggested[12] that under the growth conditions required to grow pseudomorphic $In_xGa_{1-x}N$ films, the value of S could be reduced to values close to zero, and that this promotes growth of large IHP defects. In this paper, we present the calculations which enable us to determine S for conditions in which a substantial amount of In is present in the film.

The calculations are based on the local density functional theory and employ first-principles pseudopotentials and a plane wave basis as in previous work (see, for examples, Refs. 12–18). Soft Troullier-Martins[19] pseudopotentials are employed, and the Ga $3d$ and In $4d$ electrons are treated as part of the valence band. The surfaces are modeled by repeated cells that typically contain between 20 and 50 atoms per cell, depending on the system. The atomic positions are determined by energy minimization and the plane wave cutoff is taken to be 60 Ry.

To estimate S we require values of the surface energies for the (0001) and the (10$\underline{1}$1) facets. The polar plot of surface energy $\gamma(\mathbf{n})$ is not uniquely defined for wurtzite materials such as GaN. One may add to $\gamma(\mathbf{n})$ a term proportional to $\cos\theta$, where θ is the angle between the **c** axis and **n** without changing the equilibrium shape or other thermodynamic properties.[20] Nevertheless, one may compute quantities involving the surface energies which are invariant with respect to such a transformation. S, of course, is such an invariant quantity. To compute S for GaN we use the fact that in the Ga-rich limit, the surface energies of the minimum energy reconstructions are very nearly equal for various surfaces of GaN: $\gamma(11\underline{2}0)=123$ meV/Å^2, $\gamma(10\underline{1}0)=110$ meV/Å^2, and $\gamma(001)=125$ meV/Å^2. Moreover, in the Ga-rich limit, the invariant sums of the surface energies are nearly equal: $\frac{1}{2}\{\gamma(0001)+\gamma(000\underline{1})\}=123$ meV/Å^2 and $\frac{1}{2}\{\gamma(10\underline{1}1)+\gamma(00\underline{1}\overline{1})\}=125$ meV/Å^2. Therefore, for the purpose of calculating S, we take the surface energy of the minimum energy reconstructions on the (0001) and the (10$\underline{1}$1) surfaces (the 2×2 Ga adatom and the 1×1 Ga adlayer models) to be equal to 123 meV/Å^2 and 125 meV/Å^2. This assumption, together with calculations of the relative energies of the Ga and In-terminated (0001) and the (10$\underline{1}$1) surfaces, may now be employed to estimate S.

Let us first consider growth conditions in which indium or other impurities are not present. Results for the surface energies of the relevant GaN(0001) and GaN(10$\underline{1}$1) surfaces are shown in Fig. 3. In N-rich conditions, the lowest energy structure for the (0001) surface is the 2×2 N-$H3$ adatom model,[17,21,22] and the lowest energy structure for the (10$\underline{1}$1) surface is the 1×1 Ga adatom model.[12] The value of S corresponding to these structures is 3.4. Under Ga-rich conditions, the (0001) surface of lowest energy is the 2×2 Ga-$T4$ adatom model,[17,21–23] while that of the (10$\underline{1}$1) surface is the 1×1 Ga adlayer structure.[12] In this situation S is 3.1. (For intermediate values of the Ga chemical potential, $S=3.3$.) Thus, in the absence of In or other impurities, S is larger than 3. A plot of the formation energy as a function of pit size for $S=3$ is shown in Fig. 4. In the absence of indium, or other impurities, the surface energy anisotropy is *not* large enough to enable the (10$\underline{1}$1) facets to form at the termination of the dislocation. Indeed, one finds that on impurity-free GaN(0001) surfaces, the dislocation pits forming at the termination of dislocations do not exhibit (10$\underline{1}$1)

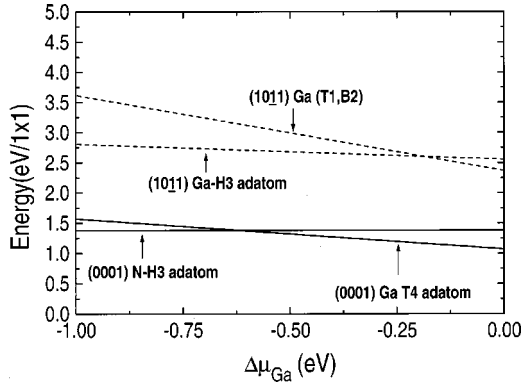

FIG. 3. Energies of the GaN(0001) and GaN(10$\bar{1}$1) surfaces. The dashed lines correspond to energies per (10$\bar{1}$1)-1×1 unit cell of the Ga adatom and the Ga adlayer structures. The area of a (10$\bar{1}$1)-1×1 unit cell is 18.6 Å^2. The solid lines correspond to the energies per (0001)-1×1 unit cell of the Ga adatom and the N adatom structures. The area of a (0001)-1×1 unit cell is 8.7 Å^2. Energies are plotted as a function of the Ga chemical potential.

facets. Instead, they are shallow pits that may be quite large in lateral extent but only a few nanometers in depth.[24,25]

Let us now consider the case of an $In_xGa_{1-x}N$ film where In is available to replace Ga atoms at the surface. As we shall see, this lowers the formation energy of the surfaces and reduces S. The change in the energy arising from the replacement of a Ga atom by an In atom depends on the relative chemical potential of the two species. Thus the change in energy (per unit cell) arising from the replacement of Ga by In is

$$\Delta E_{\mathrm{surf}} = E_0 - n_{\mathrm{sub}}(\Delta\mu_{\mathrm{In}} - \Delta\mu_{\mathrm{Ga}}),$$

where $\Delta\mu_{\mathrm{In}} = \mu_{\mathrm{In}} - \mu_{\mathrm{In(bulk)}}$, $\Delta\mu_{\mathrm{Ga}} = \mu_{\mathrm{Ga}} - \mu_{\mathrm{Ga(bulk)}}$, n_{sub} is the number of replacements per cell, and E_0 is the calculated change in energy for $\Delta\mu_{\mathrm{In}} = \Delta\mu_{\mathrm{Ga}} = 0$. We have found that when In substitutes for a Ga atom in an $S3$ site on the (0001) surface, the corresponding value of E_0 is approximately 1.1 eV. In contrast, when In substitutes for $T1$-site Ga atoms on the (000$\bar{1}$) surface, E_0 is -0.1 eV. Thus, the energy of substitution is highly site dependent. One reason for this site dependence is that the In-N bond is 11 percent longer than

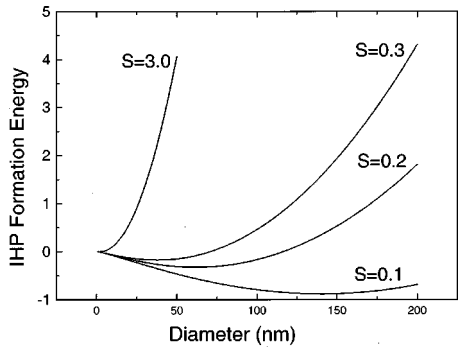

FIG. 4. Energy of the IHP as a function of its diameter for the case $S = 0.1$, 0.2, 0.3, and 3.0. For large values of S (greater than 3), the pit size is less than a few nanometers. For small values of S, the equilibrium pit size ($\sim$100 nm) and energy are very sensitive to the value of S. The energy is given in units of $10^4\gamma_0 r^2 = 0.47 \times 10^4$ eV.

TABLE I. Energy change per 1×1 cell of the (0001) surface arising from the replacement of Ga with In atoms for various surface sites. N_{sub} is the number of replacements in each 1×1 cell. The energy change is $\Delta E = E_0 - n_{\mathrm{sub}}(\Delta\mu_{\mathrm{In}} - \Delta\mu_{\mathrm{Ga}})$. Replacement of Ga atoms on the $T1$ and $B2$ sites is energetically favorable in comparison to replacement of atoms in $S3$ sites.

Surface	Reconstruction	n_{sub}	Sites	E_0 (eV)
(0001)	1×1 ideal	1	$S3$	1.09
(0001)	1×1 adlayer	2	$S3$,$A1$	0.99
(0001)	2×2 Ga vacancy	$\frac{3}{4}$	$S3$	1.44
(10$\bar{1}$1)	1×1 adlayer	2	$T1$,$B2$	0.04
(10$\bar{1}$1)	1×1 adatom	1	$H3$	0.34
(10$\bar{1}$0)	1×1 Ga-N dimer	1	$S3$	1.49
(000$\bar{1}$)	1×1 adlayer	1	$T1$	-0.13
(10$\bar{1}$1)	1×1	2	$B2$,$S3$	1.27

the Ga-N bond. Thus, there is an energetic benefit realized by the sites where the In-N bond length may relax easily to a larger value. Results obtained for a number of different sites on various surfaces are compiled in Table I. For the (0001) surface, the 1×1 adlayer structure contains Ga atoms in both the $A1$ and $S3$ sites, and the Ga-In replacement changes the energy by $\Delta E_{\mathrm{surf}}(0001\ \mathrm{adlayer}) = 0.99 - 2(\Delta\mu_{\mathrm{In}} - \Delta\mu_{\mathrm{Ga}})$ eV per 1×1 cell. For the (10$\bar{1}$1) surface, the replacement of the Ga atoms in the $T1$ and $B2$ surface sites with In atoms lowers the energy by $\Delta E_{\mathrm{surf}}(10\bar{1}1) = 0.04 - 2(\Delta\mu_{\mathrm{In}} - \Delta\mu_{\mathrm{Ga}})$ per 1×1 cell of the (10$\bar{1}$1) surface. Using these results together with the energies for the Ga-terminated surfaces, enables us to determine the energies of the In-terminated surfaces as a function of $(\Delta\mu_{\mathrm{In}} - \Delta\mu_{\mathrm{Ga}})$. Results for the surface energies of the most stable In-terminated (0001) and (10$\bar{1}$1) surfaces are shown in Fig. 5. It is clear from this plot that the energy cost of replacing a (0001) facet with a (10$\bar{1}$1) facet depends on the chemical potentials of In and Ga, and that it may be much less than in the case of the clean surface.

Only under very Ga-poor and In-rich conditions can indium be incorporated in the pseudomorphic $In_xGa_{1-x}N$

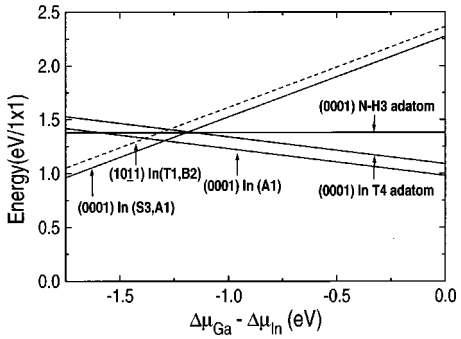

FIG. 5. Energies of In-terminated (0001) and (10$\bar{1}$1) surfaces of GaN. The dashed line corresponds to the energy per (10$\bar{1}$1)-1×1 cell of the In adlayer surface with $T1$ and $B2$ sites occupied by In atoms. The solid lines correspond to energies per (0001)-1×1 cell of various (0001) surfaces. Under In and Ga-rich conditions $(\Delta\mu_{\mathrm{Ga}} - \Delta\mu_{\mathrm{In}} > -1.25\ \mathrm{eV})$, the (0001) surface consists of In atoms in $A1$ sites. Under In-rich and Ga-poor conditions $(\Delta\mu_{\mathrm{Ga}} - \Delta\mu_{\mathrm{In}} < -1.25\ \mathrm{eV})$, the $A1$ and $S3$ sites on the (0001) surface are occupied by In atoms. The energy of the 2×2 N-$H3$ adatom structure is included for reference.

films. To quantify this notion in terms of the In and Ga chemical potentials, we performed calculations of the formation energy of substitution for an In atom replacing a Ga atom in a freestanding GaN film. In these calculations, the atoms are free to relax along the [0001] direction, but the lattice constant in the (0001) plane is kept equal to that of GaN. In this manner, we simulate the environment of an In atom in a pseudomorphic $In_xGa_{1-x}N$ film. As before, the formation energy of an In atom on the Ga sublattice may be expressed in terms of the chemical potentials of In and Ga as follows: $\Omega = E_0 - \Delta\mu_{In} + \Delta\mu_{Ga}$. Our calculations indicate that E_0 is 1.93 eV. For a dilute alloy, the In concentration x in the film is given approximately by $x = 1/(e^{\Omega/kT}+1)$. Using this relation we may determine Ω, and hence $\Delta\mu_{Ga} - \Delta\mu_{In}$, as a function of x. For example, to obtain an In concentration $x \sim \frac{1}{8}$ at a growth temperature of $kT \sim 0.1$ eV, we must have $\Delta\mu_{Ga} - \Delta\mu_{In} \sim -1.7$ eV. Thus, formation of $In_xGa_{1-x}N$ alloys is indeed obtained only under very Ga-poor and In-rich conditions. To obtain In concentrations greater than about 1%, we must have $\Delta\mu_{Ga} - \Delta\mu_{In} < -1.5$ eV.

As seen in Fig. 5, when $\Delta\mu_{Ga} - \Delta\mu_{In}$ is less than -1.5 eV, the energy difference between the In-terminated $(10\underline{1}1)$ surface and the In-terminated (0001) surface is very low. For $\Delta\mu_{Ga} - \Delta\mu_{In} < -1.25$ eV, the lowest energy (0001) surface is a structure in which an adlayer of In resides in $A1$ sites above a monolayer of In in $S3$ sites. The lowest energy $(10\underline{1}1)$ surface is the In adlayer structure with In occupying $T1$ and $B2$ sites. The calculated difference in energy between these two structures, $(\gamma_{(10\underline{1}1)}/\alpha - \gamma_{(0001)})$, is 10 meV/Å^2 and the corresponding value of S is 0.2. A plot of the formation energy of the IHP as a function of size for $S = 0.2$ is shown in Fig. 4. It is evident that the pit diameter that minimizes the formation energy ΔE may become very large ($\sim$100 nm) under these conditions, and that at this size it is quite sensitive to the precise value of S when S is small. Our results show clearly that it is energetically favorable to form $(10\underline{1}1)$ faceted pits at the termination of dislocations on $In_xGa_{1-x}N$ pseudomorphic films. Once the pit has become large, the size of the pit begins to be affected by kinetic factors such as the difference in adatom mobility and growth rates on the In-terminated (0001) and $(10\underline{1}1)$ surfaces. It is then quite plausible that the actual pit size may be larger or smaller than the size that minimizes $\Delta E(x)$. The possibility that S could even become negative cannot be ruled out. However, in that case the (0001) surface reconstructions we have considered would be unstable with respect to a complex reconstruction, perhaps involving the appearance of $(10\underline{1}1)$ ''nanofacets.''

It is important to note a special feature of the $(10\underline{1}1)$ surface. Namely, there are no $S3$ sites present on this surface. For shallower sidewalls, $\theta < 62°$, the sidewall facet would exhibit $S3$ sites as on the (0001) surface. For steeper sidewalls, $\theta > 62°$, parts of the sidewall would exhibit $S3$ sites as on the $(10\underline{1}0)$ surface (see Fig. 2). As seen in Table I, it is energetically less favorable to incorporate In atoms in the $S3$ sites on the $(10\underline{1}0)$ and (0001) surfaces in comparison to the $T1$ and $B2$ sites on the $(10\underline{1}1)$ surface. For this reason we believe the optimal sidewall facet is the $(10\underline{1}1)$ plane.

What about the possibility of IHP defects at dislocations terminating on the N-face $In_xGa_{1-x}N(000\underline{1})$ surface? Our model predicts that such $(10\underline{11})$ faceted defects should not form, because S, the surface energy term, remains large. The $(10\underline{11})$ surfaces that would be created by pit formation exhibit $S3$ and $B2$ binding sites, while the $(000\hat{\underline{1}}$ surface that would be eliminated exhibits $T1$ sites. Therefore, the energetics of In substitution are not conducive to the replacement of the $(000\underline{1})$ surface by the $(10\underline{11})$ facets, and so $(10\underline{11})$ faceted dislocation pits are not expected to form in growth on the $In_xGa_{1-x}N(000\underline{1})$ surface.

In summary, we have performed calculations for a number of low-index In-terminated GaN surfaces and have shown that In behaves as a differential surfactant, reducing the energy of the $(10\underline{1}1)$ surface relative to the (0001) surface. This effect promotes the formation of large $(10\underline{1}1)$ faceted dislocation pits on (0001) surface of $In_xGa_{1-x}N$.

We are grateful to Linda Romano for valuable discussions.

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