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Research Status of GaN Film Growth

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Abstract: This paper introduces the important application fields, growth methods and molecular dynamics research methods of GaN. Due to the lack of homogeneous substrate, GaN film growth is limited and the crystal quality is poor. At present, heteroepitaxial GaN has some problems, such as high fault density, large residual stress and uneven thickness. The intermediate AlN buffer layer is used to reduce the lattice mismatch and thermal expansion coefficient mismatch between GaN film and substrate. Meanwhile, the growth mechanism of GaN is not well understood. In addition, molecular dynamics simulation is an effective tool to study GaN growth, which can reveal the growth process of GaN film and the evolution of dislocation from a microscopic perspective. The research of this work can provide reference for the next step of GaN film growth.

1. Introduction

Gallium nitride (GaN), as an important semiconductor, has material properties such as wide band gap, high breakdown voltage and high electron mobility [1]. In the past few decades, GaN materials have been widely used in ultraviolet light-emitting diode (LED), high electron mobility transistors (HEMTs) and other optical electronic devices [2]. There are many techniques for the preparation of GaN films, mainly including metal organic chemical vapor deposition (MOCVD) [3], magnetron sputtering, hydride vapor phase epitaxy (HVPE) and molecular beam epitaxy methods (MBE) [4]. MOCVD and magnetron sputtering are suitable for large-scale production, while MBE methods are usually limited to experimental studies.

III nitrides can be grown in wurtzite and sphalerite phases; the most commonly used and stable crystalline phase is wurtzite. Wurtzite structure has different surface properties and growth kinetics along <0001> and <000-1> directions [5]. In addition, due to the asymmetry of wurtzite phase inversion along the C-axis, GaN crystals have strong polarity in the C-axis direction, which leads to strong spontaneous and piezoelectric polarization fields. The polarization field of the N-pole GaN material creates a natural back barrier that moves the two-dimensional electron gas (2DEG) towards the grid, enhancing the 2DEG constraint and easing the difficulty of achieving ohmic contact. The channel thickness of N-polar HEMTs can be reduced to improve electrical performance without sacrificing 2DEG density.

So far, in the experiment and practical production application, the most important is to choose the polar plane (0001)/c plane as the growth surface of GaN film preparation, the prepared GaN film usually has Ga polarity. At present, the research on GaN film growth generally focuses on GaN and heterostructure of Ga pole. However, there are few studies on the epitaxial growth of N-polar

GaN materials. However, reverse polarization in the n-polar nitride structure can be used in many device structures. The direction of the polarization field is particularly advantageous for enhanced mode transistors and high scale GaN transistors. In addition, the N-pole surface is more reactive and suitable for sensor applications. The breakdown voltage of N-polar GaN HEMTs is greater than 2000V, and the power increase efficiency (PAE) is greater than 70% [6]. Therefore, N-pole GaN materials play a very important role in the structure of high electron mobility field effect tubes. Compared with the GA-polar AlGaN/GaN high-electron mobility field effect tube structure, the N-polar AlGaN/GaN high-electron mobility field effect tube structure has the opposite direction of spontaneous polarization and piezoelectric polarization effect. Therefore, N-polar GaN based materials are worth exploring and studying.

2. Problems existing in GaN film growth and solutions

Due to the lack of suitable single crystal substrates, sapphire and Si are used as substrates. Due to the large lattice mismatch and thermal expansion difference between these materials and GaN films, it is difficult to directly grow high-quality single crystal GaN on these substrates. Lattice mismatch is a problem that cannot be ignored, which will lead to high dielectric constant and spiral dislocation density, resulting in large residual stress in the film, and then lead to obvious cracks in the annealing process of epitaxial GaN. In addition, the film will also produce a large number of holes, gaps, impurities, stacking faults and other defects. A high dislocation density will generate a large number of non-radiative recombination centers, thereby reducing the optical and electrical properties of GaN-based devices [6]. In addition, these defects are fatal to the reliability and longevity of electronic optics. Interspersed dislocations and vacancy defects are known to generate additional current paths, and current leakage of electronic devices through the tunneling process at low forward bias may be caused by the higher dislocation and vacancy defect density in multiple quantum Wells in leds. Therefore, how to reduce the defects such as dislocation and vacancy in GaN films has become an important proposition in the preparation of GAN films. In addition, in current studies, the stress in GaN films caused by the mismatch of lattice constants and thermal expansion coefficient between substrate and GaN films is still a critical problem, which is considered to be the main factor hindering the further development of efficient GaN-based optoelectronic devices.

To reduce the lattice and thermal expansion mismatch between the epitaxial GaN layer and the substrate, a variety of intermediate buffer layer techniques have been used, including GaN, MoS_2, AlGaN, graphene [7], and AlN [8] deposited at low temperatures. So far, AlN buffer layer is considered to be the best and most commonly used intermediate buffer layer for GaN film growth, because it has the same lattice structure and smaller lattice mismatch with GaN. Therefore, when growing GaN films, choosing AlN as buffer layer can reduce the difference of thermal expansion coefficient and lattice mismatch between GaN and substrate, so as to obtain GaN films with better crystal quality. In addition, GaN has good wettability, which allows the film to be grown in two dimensions, thus obtaining high quality GaN epitaxial layer. When the sputtering AlN nucleation layer is used as the intermediate buffer layer, the substrate can be effectively protected from impurities produced by the decomposition of high temperature substrate. This technique can reduce the dislocation density in GaN films, resulting in the growth of high-quality GaN films. Wang et al. [9] used MOCVD epitaxial growth of GaN films to study the effects of different V-III ratios and growth temperatures on the surface morphology and internal stress of GaN films. Although there have been many studies on GaN epitaxial growth, the dislocation distribution and stress evolution in the epitaxial layer during GaN growth are not very clear. Therefore, it is of great significance to understand the growth mechanism and microstructure of GaN thin films on the nanoscale by using molecular dynamics simulation method.

3. Molecular dynamics simulation of thin film growth

In recent years, molecular dynamics simulation (MD) has been widely used to predict and investigate the epitaxial growth processes of various thin films. MD can intuitively analyze the growth process of various films and understand their atomic scale behavior. Even with in situ transmission electron microscopy (TEM), it is difficult to monitor the details of microstructure and defect evolution at atomic scale. On the other hand, MD can provide the motion trajectory of all atoms and directly observe the entire film growth process from the microscopic atomic scale, thus revealing the evolution mechanism of the film. Some relevant studies are as follows:

Hassan Amini et al. [10] used MD simulation to study the effects of different substrate temperatures and incident energy on the crystallinity of Ti-TiN multilayers and the evolution of atomic microscopic stress in them. Chen [11] studied the surface structure formation mechanism and film properties of amorphous TiO_2 films under different incident energies of titanium atoms. Camas et al. [12] studied the epitaxial growth of cubic $InxGa_{1-x}N$ layer on GaN(001) buffered substrate, and investigated the influence of substrate temperature, flux ratio of In, Ga and N, and concentration of In on dislocation density and crystal quality of cubic $InxGa_{1-x}N$ thin films. Zhang et Al. [13] used MD method to explore the effects of GaN substrate surface, growth temperature and N:Al flux ratio on the surface morphology and crystallinity of AlN films. Although Liu et al. [14] simulated the epitaxial growth of GaN film on AlN substrate and studied the effects of different Ga:N flux ratio and growth temperature on the crystal structure of the film, different substrate surface is an important factor affecting the growth of the film. At present, the growth mechanism of GaN film, the influence of polar and non-polar growth surfaces of AlN substrate on GaN film growth, and the evolution process of dislocation and stress in the film are still unclear. Therefore, it is necessary to investigate the epitaxial growth process of GaN films on AlN substrates with different polar surfaces at the atomic scale.

4. Growth parameters of GaN

The polarity of the III-N group is an inherent property, and its polarity is closely related to growth conditions and deposition mode. Termination of GaN wurtzite crystals at the top of Ga or N atoms is called Ga-pole face and n-pole face, and this type of growth is called C-site GaN. The relevant literature shows that in addition to the base temperature, incident energy, flux ratio, incident Angle, deposition rate, etc., the substrate with different crystallographic planes is also an important factor affecting the final quality of the film. At present, for example, GaN films grown on N-pole AlN substrates have N polarity, while GaN films grown on N-pole AlN substrates by heteroepitaxy have Ga polarity. The polarity of GaN film may also be related to the thickness of AlN buffer layer.

5. Research prospect

Although it is confirmed that growth temperature and substrate surface are important factors affecting the surface morphology, surface roughness, crystal structure, dislocation density, dislocation distribution and atomic stress evolution of GaN film, it is necessary to study the effects of more growth parameters on GaN film growth in the future.

(1) Relevant studies show that in addition to these two influencing factors, atom incident energy, flux ratio, deposition rate and other factors have a significant impact on the deposition process, which is worth exploring in future research work.

(2) Some researchers have studied the effect of V/III ratio on GaN films grown at high temperature by using the two-step growth method, and concluded that GaN films prepared by the two-step method have more compressibility and strong tensile resistance. However, no one has explored the changes of microstructure and stress of thin films in the two-step growth process from the perspective of molecular dynamic simulation. So that's a good point to look at.

(3) The use of patterned substrate surfaces, such as cylindrical and conical substrates, will also affect the density of the film and promote the bending of the dislocation. This point also needs attention when preparing GaN films. Therefore, more influencing factors need to be studied in the future, especially when growing on substrates with different crystal orientation, which will greatly contribute to improving the quality of epitaxial GaN films.

6. Conclusion

Due to the lack of homogeneous substrate, GaN film growth is limited and the crystal quality is poor. At present, heteroepitaxial GaN has some problems, such as high fault density, large residual stress and uneven thickness. In order to reduce the lattice mismatch and thermal expansion coefficient mismatch between GaN film and substrate, an intermediate AlN buffer layer is used. At the same time, there are few studies on the growth of N-pole GaN. In addition, molecular dynamics simulation is an effective tool to study GaN growth, which can reveal the growth process of GaN film and the evolution of dislocation from a microscopic perspective. At present, the growth mechanism of GaN film, the influence of polar and non-polar growth surfaces of AlN substrate on GaN film growth, and the evolution process of dislocation and stress in the film are still unclear. Therefore, it is necessary to investigate the epitaxial growth process of GaN films on AlN substrates with different polar surfaces at the atomic scale. Finally, the research of GaN film growth is prospected. The research results of this paper provide guidance for GaN film growth research.

References

[1] J. Wu, When group-III nitrides go infrared: new properties and perspectives, J. Appl. Phys. 106 (2009) 11101.

[2] H. Amano, N. Sawaki, I. Akasaki, Metalorganic vapor phase epitaxial growth of a high quality GaN film using an AlN buffer layer, Appl. Phys. Lett. 48, 353 (1986).

[3] Y. Sun, K. Zhou, et al, Room-temperature continuous-wave electrically injected InGaN-based laser directly grown on Si, Nat. Photonics 10 (2016) 595–599.

[4] X. Zhu, J. Wu, et al. Free-standing GaN grown by HVPE with sputtered AlN buffer on GaAs substrate, J. Cryst. Growth. 540 (2020) 125637.

[5] Y. F. Li, X. T. Hu, et al., The role of AlN thickness in MOCVD growth of N-polar GaN, J. Alloy. Compd. 884 (2021) 161134.

[6] S. Kolluri, D.F. Brown, et al., RF performance of deep-recessed N-polar GaN mis-hemts using a selective etch technology without ex situ surface passivation, IEEE Electron. Device Lett. 32 (2011) 134–136.

[7] Y. Zeng, J. Ning, J. C. Zhang et al, Raman Analysis of E 2 (High) and A 1 (LO) Phonon to the Stress-Free GaN Grown on Sputtered AlN/Graphene Buffer Layer [J]. Appl. Sci. 2020, 10, 8814.

[8] S. M. Kang, et al. Influence of AlN buffer layer thickness and deposition methods on GaN epitaxial growth, Thin Solid Films 517 (2009) 5057–5060.

[9] Y. Wang, et al. Growth of high-quality nitrogen-polar GaN film by two-step high-temperature method, Thin Solid Films 752 (2022) 139246.

[10] H. Amini, et al. A molecular dynamics simulation of Ti-TiN multilayer deposition on FeCrNi (001) alloy substrate, Vacuum 193 (2021) 110519.

[11] X. Chen, Y. W. Wang, et al. Molecular dynamics study of the effect of titanium ion energy on surface structure during the amorphous TiO_2 films deposition, Appl. Surf. Sci. 345 (2015) 162–168.

[12] C. Camas, J. E. Conde, et al. Molecular dynamics simulation of cubic $In_xGa_{(1-x)}N$ layers growth bymolecular beam epitaxy, Comput. Mater. Sci. 193 (2021) 110387.

[13] L. B. Zhang, H. Yan, et al, Molecular dynamics simulations of AlN deposition on GaN substrate [J]. Mol. Simul. 117 (13) (2019) 1758–1767.

[14] K. Liang, X. Sun, et al. The investigation of molecular beam epitaxy growth of GaN by molecular dynamics simulation, Comput. Mater. Sci. 173 (2020).