The methods of Mg-doped GaN-based p-type semiconductors

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Abstract. This article mainly discusses the disadvantages of the third-generation semiconductor material based on GaN and points the ways of optimization and development. The P-type doping optimization method is especially focused. As the core element of P-type doping, Mg element has its advantages and disadvantages in research and use, and some improvement methods are pointed out. In addition, the principles of several specific P-type doping methods, mainly including polarization-induced doping, Mg-delta doping, superlattice doping, and Mg-In co-doping are discussed.

Keywords: GaN semiconductors; P-type doping; Mg-delta doping; superlattice doping.

1. Introduction

Due to intrinsic defects present in third-generation semiconductor GaN, the material exhibits a heightened concentration of free electrons. Hence, researchers are diligently enhancing material growth techniques to bolster material performance. The elevated concentration of intrinsic defects in GaN stems from its growth process occurring in a nitrogen-rich environment, where nitrogen is in gaseous form and susceptible to desorption due to high temperatures. Furthermore, the weak chemical bond between gallium (Ga) and nitrogen (N) prevents the formation of a stable bond, resulting in nitrogen vacancies—these vacancies are intrinsic defects. Consequently, the outermost electrons of Ga atoms easily become free electrons, facilitating their unrestricted movement within the material and inducing an overall electronegative state. Remarkably, even without impurity doping, the material exhibits N-type doping characteristics. Ordinarily, the electron concentration in the material remains below 10^{10} cm^{-3}, rendering the material highly resistant [1]. Only when the electron concentration surpasses 10^{10} cm^{-3} does the material achieve conductivity. In the realm of semiconductor devices, the simultaneous presence of P-doping and N-doping is essential for creating a complete device capable of serving as an electrical or optical component. Consequently, enhancing P-type doping in semiconductor materials becomes imperative, particularly in wide bandgap GaN semiconductor materials—an avenue of research that holds great importance.

2. The cons of Mg doping in GaN-based materials

2.1. The atomic memory effect of Mg

The atomic memory effect of Mg is focused during the P-type doping process. This is because when CP_2Mg and NH_3 are reacted in the reaction chamber using MOCVD technology, some reactants do not form the replacement atoms of Ga atoms, but are adsorbed on the side wall of the reaction chamber after condensation, and the adsorbed Mg Atoms are re-released to affect subsequent growth. Its characteristics will require high geometric design and growth pressure control of the reaction chamber. The lower the pressure, the weaker the memory effect of Mg atoms. [2]Furthermore, Mg atoms have a small metal radius and are active. During the reaction process, the furnace wall will cover Mg atoms, and Mg atoms will diffuse into the subsequently grown material during subsequent growth. Under normal circumstances, after a growth experiment of Mg doping is completed, the reaction chamber will be flushed with high-temperature airflow, so as to achieve the cleaning effect.

2.2. The floating and diffusion effect of Mg

In general, the floating characteristic is one of the processes of the memory effect of Mg atoms. Floating or attaching of Mg atom in the subsequent growing environment with other doped materials, it will diffuse or run out from the attached sidewall or furnace and enter the subsequent in the grown material, thus affecting the doping effect.

2.2.1. Diffusion effect

Because Mg atoms have a very strong diffusion effect, Mg atoms will diffuse downward in the P-type material. Normally, the lower layer is GaN doped with Si type. Because there are many vacancies in the GaN material, voids or other forms of defects are formed. Mg uses the gaps or vacancies of these defects to gradually obtain high diffusion energy at high temperature due to the diffusion of atoms requires a certain temperature, and then diffuses toward the N-type doped material, making the material become Mg-Si co-doped.

2.3. The self-compensation effect of Mg

As the doping concentration of Mg atoms increases (substitution doping), there is a difference in unit cell size between Mg atoms and Ga atoms, which in turn forms periodic atomic arrangement or lattice distortion of atomic morphology, resulting in changes in the overall lattice constant of the material. . Lattice distortion introduces distortion energy, which in turn causes many defects to form in the material. Distortion energy reduces the conditions for the initiation of defect energy, thereby increasing the concentration of defects. After the defect is formed, it is contrary to the purpose of Mg atom doping (to form a hole). After the defect is formed, the defect becomes a bound fixed negative charge (equivalent to an electron). Negative charges (defects) and positive charges (holes) cancel and neutralize each other, so that the more Mg impurities in the material are doped, the less the material will exhibit p-type doping characteristics. When the Mg impurity exceeds a certain level, the more Mg atoms are doped, the lower the activation efficiency of the Mg impurity is.

2.4. Mg-H compound

Mg atoms are doped into the GaN material, and the Mg atoms replace the positions of the Ga atoms, because the outermost layer of Mg has two electrons, while the outermost layer of Ga has three electrons. After the substitution of Mg, one electron is paired less, and then the material will capture an electron from the environment to form a stable structure (bonding) of 8 electrons. Therefore, Mg presents electronegativity in the environment, and an electropositive vacancy needs to be formed in the environment and can make the material exhibit electrical neutrality. Therefore, good P-type conductivity characteristics are formed in the Mg-doped GaN material. The introduction of the H atom provides a free electron, which combines with the Mg atom. The Mg atom does not need to capture electrons from the environment, so that the material cannot form holes, and thus cannot form P-type conductivity. Therefore, the Mg-H complex reduces the efficiency of Mg doping, thereby failing to form a high concentration of holes. High temperature or ion bombardment attempts to break the chemical bonds of the Mg-H complex so that the Mg atoms can be activated to generate holes.

3. The methods of Mg-doping in GaN-based semiconductors

During the growth process of the material, if the lattice constants of the atoms in the upper layer and the atoms in the lower layer do not match, a piezoelectric field will be generated between the atoms in the upper layer and the atoms in the lower layer (the material belongs to the piezoelectric material). The polarized dipole strength is not the same in materials, and then a sudden change in the polarized electric field is formed at the interface (two adjacent atomic layers at the interface). In electrokinetics, there is a polarized electric field, and a polarization-induced fixed charge is formed at the interface. The formed fixed negative charge will induce the appearance of holes, and then form the characteristic of P-type conductivity. Even, Mg doping is not required, only atoms need to form

a polarization-induced charge at the interface between the two (holes can be formed without Mg doping). Based on this principle, the AlGaN material with a gradual change in the AI composition will form a polarized electric field between each atomic layer and the previous atomic layer due to the difference in the Al composition, thus forming a two-dimensional surface charge. Stacked in the material is a 3D controllable polarization-induced charge [3-4].

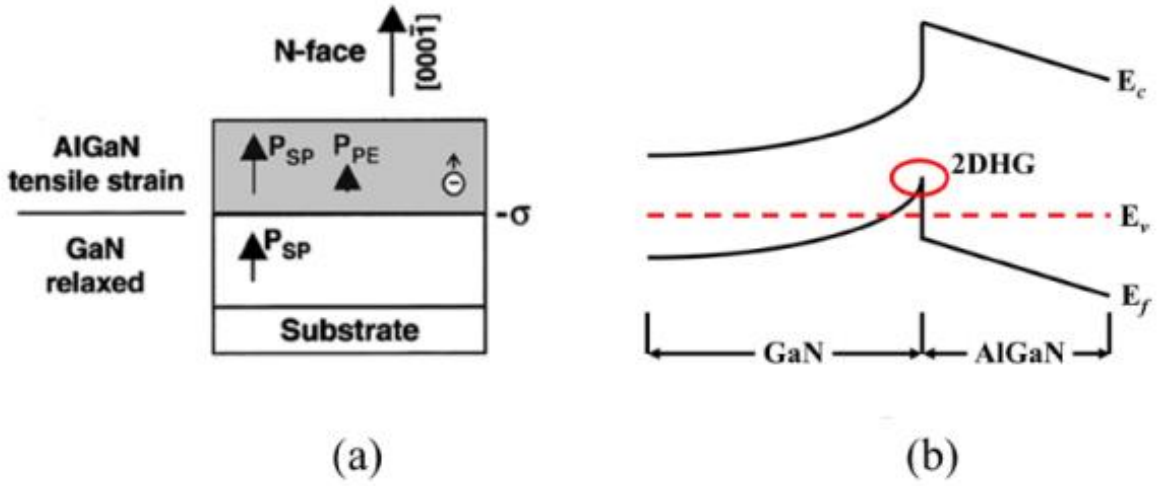


Fig 1. Nitrogen polarity AIGaN/GaN heterojunction polarization effect (a) and its energy band structure schematic diagram (b) as shown above.

Under normal circumstances, during the material growth process, in each growing layer of GaN unit cells, some Ga positions are replaced by Mg atoms. However, in Mg-delta doping, the supply of Ga atoms is suddenly stopped, and then changed to all Mg atoms, which is actually realized as the complete replacement of Ga atoms by Mg atoms. Therefore, in some areas, Mg atoms show a high concentration, breaking the the lattice structure of GaN and forms dislocations. According to inertia and principal, dislocations extend upward during the growth process, causing the density of defects such as dislocations to decrease under the action of its blocking, because the traditional periodic structure is broken. The original periodic dislocation movement or upward extension process is blocked, the concentration of dislocations is reduced, and the trapping effect of dislocations on vacancies is reduced. Due to the reduction of defects such as dislocations, the negative charges formed by the defects will form a compensation trap. The combination of these defects and Mg atoms will form fixed bound defect bodies. Defects make it difficult for Mg impurities to activate. Therefore, reducing the existence of defects can reduce the binding of Mg impurities, and also reduce the formation of complexes between impurities and Mg, such as (Mg-H complexes) to improve the activation efficiency of Mg impurities. During the growth process, high-concentration Mg doping presents discontinuous doping, and this high-concentration doping forms dislocations and suppresses the self-compensation defects of Mg. In turn, the hole concentration is greatly increased [5].

The doping method of the superlattice makes the energy band of the material bend (i.e. normally, the energy band is linear) so that the fermi level of the material is higher than the energy level of Mg doping. Due to the lattice mismatch when the two are formed, a piezoelectric polarization electric field will be formed, and the piezoelectric polarization electric field will bend the energy band. Because the fermi energy level will not be affected by the piezoelectric polarization electric field, the doping of atoms such as MgAI bends some energy bands, making the energy bands in some regions of the material lower than the fermi level, the activation energy of Mg impurities is reduced, making the material easier to activate.

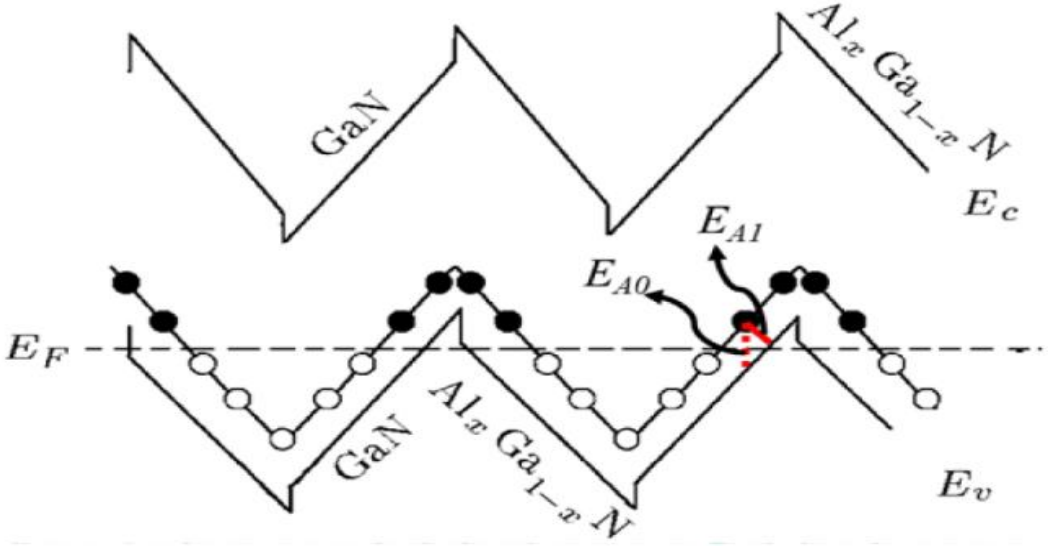


Fig 2. The energy band structure of superlattice materials doped with AIGaN/GaN as shown above.

The purpose of Mg-In co-doping is to reduce the forbidden band width between fermi energy level and valence band.

In general, the energy level of GaN is higher than the fermi energy level, because electrons need to transition from the fermi energy level to the GaN energy level to form holes, and the initial transition energy band width is wide (more energy is required to excite electronic transitions), Because the wider the width, the more energy is required. Mg atom doping is introduced because the lattice constant of in atoms is larger than that of Ga atoms. In semiconductors, the larger the lattice constant, the narrower the forbidden band width. Doping In atoms into the GaN material will reduce the overall energy band of the material. The transition of Mg atoms becomes easier and the required thermal energy is reduced, thus making Mg doping easier to activate.

4. Conclusion

To sum up, the pros and cons of the third-generation semiconductor material based on GaN, and the approaches of optimization and development and the P-type doping to GaN optimization methods are especially discussed. As the core element of P-type doping, Mg element are introduced and some improvement methods are pointed out. In addition, the principles of several specific P-type doping methods, mainly including polarization-induced doping, Mg-delta doping, superlattice doping, and Mg-In co-doping are discussed. Those methods increased the efficiency of P type doping of GaN, but their disadvantages are clear such as precise temperature and geometry control are needed.

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