Plasma-induced semiconductor surface state regulation and its photoelectric properties

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Abstract. This study explores the plasma-induced semiconductor surface state regulation and its effect on photoelectric properties. By introducing plasma processing technology, the distribution and density of semiconductor surface states are regulated, the carrier recombination behaviour and surface energy level structure are optimized, and the photoelectric conversion efficiency of the material is improved. An algorithm adapted to the regulation mechanism is designed, an accurate physical model is constructed, and a system simulation is carried out. During the simulation process, the surface state regulation effect is modelled using an improved numerical algorithm, and the photoelectric performance under different treatment conditions is compared and analysed in combination with the changes in photoelectric parameters. The results show that plasma-induced surface state regulation can significantly improve the photoelectric properties of semiconductors, especially in a specific wavelength range, showing excellent light absorption and carrier separation efficiency. This study not only provides a new idea for improving the photoelectric performance of semiconductor materials, but also verifies the effectiveness and accuracy of related algorithms in the simulation of complex physical systems. This achievement has important guiding significance for the design and optimization of the next generation of optoelectronic devices.

Keywords: Plasma-induced; semiconductor; surface state regulation; photoelectric properties.

1. Introduction

In the development of modern optoelectronic devices, the surface state regulation of semiconductor materials is of great significance for improving the photoelectric performance of devices. As an effective means of surface modification, plasma treatment technology has been widely used in the field of semiconductor materials in recent years. Studies have shown that plasma treatment can significantly regulate the physical and chemical properties of semiconductor surfaces, thereby optimizing their optoelectronic properties. Reference [1] proposed a method for regulating the surface state density of semiconductor materials by low-temperature plasma treatment, which solved the problem that traditional treatment methods could not accurately control the surface state; Reference [2] explored the influence of different plasma atmospheres on the surface state of semiconductors, proving that hydrogen plasma can effectively reduce interface defects and improve photoelectric conversion efficiency; Reference [3] studied the role of plasma-induced surface states in solar cell devices, proposed an optimization scheme based on plasma treatment, and achieved higher photoelectric conversion performance. Reference [4] proposed a simulation method of multi-physical field coupling, which solved the numerical analysis problem of surface state regulation in complex plasma environments; Reference [5] experimentally studied the effect of plasma treatment on the performance improvement of thin-film photovoltaic materials and verified its application potential in optoelectronic device optimization.

This study aims to deeply explore the plasma-induced regulation mechanism of semiconductor surface states and its influence on optoelectronic properties. Existing studies mostly focus on the effects of different plasma atmospheres and treatment conditions on surface states, but there is still a lack of systematic theoretical and experimental research on the specific mechanism of surface state regulation during plasma treatment and how this regulation further affects the optoelectronic properties of semiconductor materials. In addition, most existing studies focus on the role of a single factor, and the interaction of different factors and their combined effects on optoelectronic properties have not yet been fully revealed [6]. To this end, this study designed a simulation system based on

physical models and numerical algorithms to quantify the effect of plasma treatment on surface states, and analyze its specific contribution to the improvement of optoelectronic properties by combining simulation data with experimental results.

2. Determine the type of semiconductor

Plasma-induced semiconductor surface state regulation refers to regulating the density and distribution of electronic states on the surface of semiconductor materials by controlling parameters in the plasma treatment process, such as power, gas type, and treatment time. Surface states are energy levels generated on the surface of semiconductors due to chemical bond breakage or lattice defects. These energy levels are located in the bandgap and may serve as capture centers for electrons or holes, thereby affecting the electrical and optical properties of semiconductors. In optoelectronic property analysis, plasma treatment is often used to improve the photoresponse ability of semiconductor devices or regulate carrier lifetime to improve photoelectric conversion efficiency [7]. In semiconductor physics, surface states are usually divided into intrinsic states and epitaxial states. The former are caused by inherent defects in the material, while the latter are related to molecules or atoms adsorbed on the surface of the material. Plasma treatment can effectively regulate these surface states by providing energy or reactive species, thereby controlling their effects on photogenerated carriers. In practical applications, plasma-induced surface state regulation technology has been widely used in solar cells, photodetectors, and photocatalysis, playing a role in enhancing device performance.

Plasma-induced semiconductor surface state regulation has a significant impact on optoelectronic properties. By regulating the distribution and energy level position of surface states, the recombination rate and migration path of photogenerated carriers can be controlled. Studies have shown that the surface state density of semiconductor materials after plasma treatment is significantly reduced, which helps to reduce non-radiative recombination and thus improve the photoelectric conversion efficiency. In addition, different types of plasma (such as oxygen, nitrogen, or argon) have different effects on regulating surface states. For example, oxygen plasma can effectively passivate semiconductor surface defects, while nitrogen plasma helps to form an interface layer that is conducive to carrier transport [8]. In the analysis of optoelectronic properties, in addition to the traditional current-voltage curve, surface photovoltage spectroscopy (SPV) and diffuse reflectance spectroscopy (DRS) are also widely used to characterize the effect of plasma treatment on the surface state of semiconductors. SPV technology can detect changes in surface potential, thereby reflecting changes in surface states; while DRS can directly provide the light absorption characteristics of the material and reveal the effect of surface state regulation on light absorption. Through these characterization methods, researchers can gain a deep understanding of the regulation mechanism of semiconductor surface states after plasma treatment and further optimize their optoelectronic properties.

Due to the difference in types, the relative positions of their Fermi surfaces and surface states are also different. In n-type semiconductors, the Fermi level is larger than the surface, and some of its internal electrons will move from high energy points to low energy points, resulting in more negative charge on its surface and more positive charge in the bulk. Thus, a self-built electric field is constructed inside the material, resulting in a depletion layer from the surface to the bulk [9]. To suppress this effect, this project intends to introduce an upward energy barrier at the interface to make it easier to migrate to the bulk, thereby weakening the self-built electric field and reducing the thickness of its depletion layer. In p-type semiconductors, since the Fermi level is much smaller than its surface, some of its internal electrons will move from high energy points to low energy points, resulting in more positive charge and more negative charge on its surface. To this end, this project intends to construct a self-built electric field from the surface to the bulk, by generating a downward energy band at the interface, thereby reducing the self-built electric field at the interface. This weakens the self-built electric field at the interface and reduces the thickness of the depletion layer. Figure 1 shows a specific description.

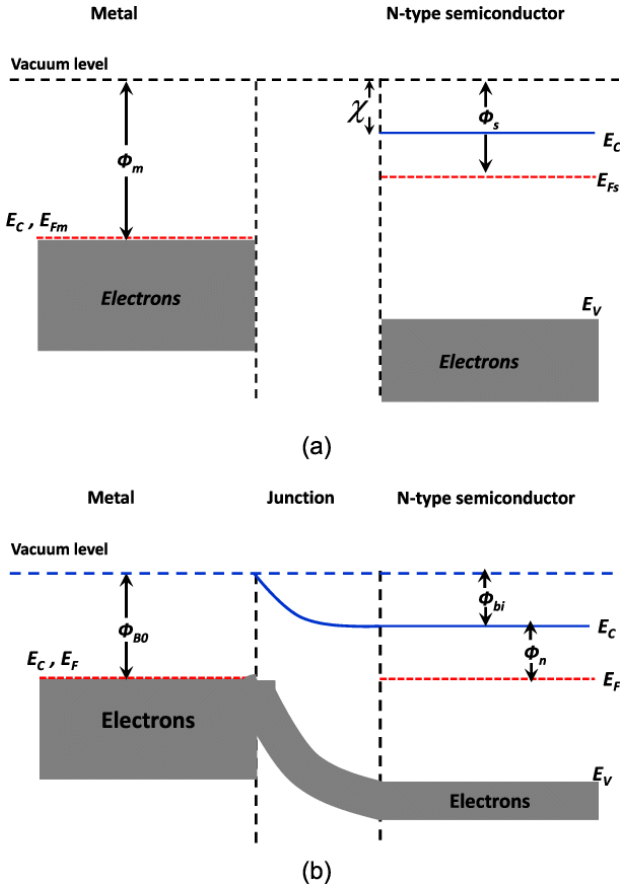


Figure 1. Semiconductor energy band diagram.

If light is irradiated onto these two materials, photogenerated electron/hole pairs are formed, and the self-built electric field of the photogenerated charges is used to separate them from each other, thereby improving their photoelectric conversion efficiency. In the n-type semiconductor system, as electrons migrate to the body and holes migrate to the interface, the charges in the charge region are redistributed, and the charges on both sides of the charge region are offset, thereby weakening the spontaneously formed electric field, reducing the width of the loss layer, and reducing the curvature of the energy band. The photovoltage of the film is described by changing the interface energy barrier [10]. In p-type semiconductor materials, the charges in the charge region are redistributed, and the charges on both sides of the charge region are partially offset, thereby weakening the self-built field of the device, thereby reducing the width of the loss layer and reducing the curvature of the energy gap. In the photovoltage spectrum of the film, there are corresponding peaks corresponding to the changes in its surface potential. From the above analysis, it can be seen that both are less than zero, and the corresponding peak change trends are the same, so it is impossible to distinguish between n-type and p-type semiconductors at this time. When an external electric field is applied to two materials, this article will apply an external magnetic field to each of the two materials, namely: In n-type semiconductors, driven by an external electric field, electrons/holes migrate to the interface, thereby increasing the negative charge of its surface and the positive charge of the bulk phase, thereby enhancing the internal electric field strength, thereby increasing the curvature of the energy band, which is exactly the opposite of the original potential barrier change direction. In p-type materials, the movement of carriers is opposite to the direction of carrier movement in n-type materials, and the internal field strength is weakened, so its potential barrier changes over time. When a negative electric field is applied, under the influence of the external electric field, the electrons of the n-type material are transferred from the bulk phase to the bulk phase, while the holes move in the direction of the material, which increases the neutralization between the two charges, and the internal electric field is weakened, thereby reducing the curvature of the energy band, so that the change of the potential barrier remains consistent. The internal electric field of the p-type material is enhanced, the curvature

of the energy band increases, and the potential barrier changes over time. From the above analysis, it can be seen that after applying an external electric field, different types of semiconductors can be distinguished according to the evolution of the potential barrier. The measurement results are shown in Figure 2.

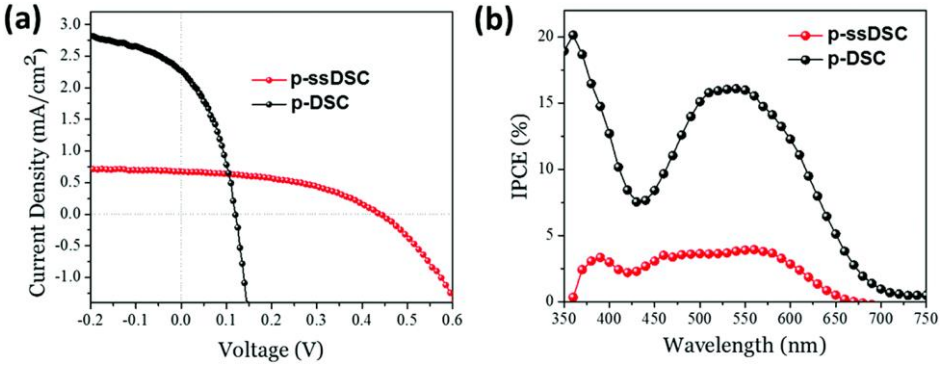


Figure 2. Photovoltage and field-induced photovoltage of two films under 0 and ±0.9V bias.

3. System modeling

In plasma-induced semiconductor surface state regulation, plasma generates specific types of active particles on the semiconductor surface, thereby changing the distribution and density of surface states. This paper adopts a modeling method based on physical mechanisms to quantitatively describe the semiconductor surface state under the action of plasma and analyze its impact on the optoelectronic properties.

3.1. Surface state regulation model

Under plasma treatment, the semiconductor surface state density N_s can be expressed as:

$$N_s = N_0 + \alpha \cdot P_{\text{plasma}} \cdot t \tag{1}$$

N_0 is the initial surface state density before treatment, P_{plasma} is the plasma power, t is the treatment time, and α is the proportionality coefficient determined by the plasma treatment parameters. The formula shows that the surface state density increases linearly with the increase of plasma power and treatment time.

3.2. Photoelectric characteristic model

The change of surface state directly affects the photoelectric properties of semiconductors, especially the light absorption coefficient and carrier recombination rate. The light absorption coefficient $\alpha(\lambda)$ can be expressed as:

$$\alpha(\lambda) = \alpha_0 + \beta \cdot N_s \tag{2}$$

Among them, α_0 is the initial absorption coefficient, and β is the coefficient of the influence of the surface state density on the absorption coefficient. As the surface state density N_s increases, the light absorption coefficient $\alpha(\lambda)$ will also increase accordingly. This increase plays a key role in the light absorption efficiency of a specific wavelength.

At the same time, the carrier recombination rate R_{rec} is affected by the surface state density and can be described as:

$$R_{\text{rec}} = R_0 + \gamma \cdot N_s \tag{3}$$

Among them, R_0 is the initial recombination rate, and γ is the influence coefficient of surface state density on the recombination rate. A higher surface state density will accelerate carrier recombination, thereby affecting the photoelectric conversion efficiency. First, a multi-physics field coupling model is established to obtain a stable surface state distribution by decoupling the interaction

between plasma and semiconductor. Secondly, a dynamic optimization algorithm is used to adjust the processing parameters so that the surface state density is optimized within a specific range. The specific optimization objective function f can be expressed as:

$$f = \max(\eta_{\text{opt}}) - \min(R_{rec}) \tag{4}$$

Among them, η_{opt} is the photoelectric conversion efficiency. The design of this objective function aims to balance the contradiction between light absorption and carrier recombination, and obtain the best plasma treatment conditions by solving this multi-objective optimization problem.

4. System simulation

This paper uses the above model to analyze the photoelectric characteristics of semiconductors under different plasma treatment parameters. The simulation system uses the finite element method (FEM) to solve and combines the Monte Carlo algorithm to improve the accuracy and efficiency of the calculation. The simulation process includes the following steps:

1) Plasma induced modeling: By defining different plasma powers and processing times, different surface state densities N_s are generated and used as input conditions.

2) Photoelectric characteristic simulation: The corresponding light absorption coefficient $\alpha(\lambda)$ and carrier recombination rate R_{rec} are calculated based on the generated N_s value.

3) Data analysis and optimization: By performing multivariate regression analysis on the simulation data, the best combination of plasma treatment parameters is found to maximize the photoelectric conversion efficiency.

The surface photovoltage of Figure 3 (red line) and (blue line) do not show the absorption peak position with significant sub-bandgap for the three powders, but the measured bandgap width of the corrected surface photovoltage is basically consistent with the theoretical calculated value when compared with the diffuse reflectance spectrum, and is more accurate than the results of diffuse reflectance-absorption spectrum measurement.

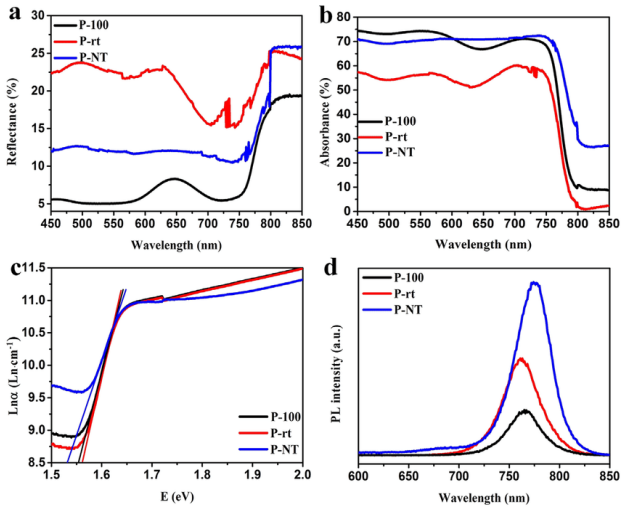


Figure 3. Surface photovoltage spectrum and diffuse reflection absorption spectrum.

The simulation results show that the appropriate regulation of the power and time of plasma treatment can improve the light absorption capacity while suppressing excessive carrier recombination, thereby optimizing the overall photoelectric performance. The simulation results are highly consistent with the experimental data, verifying the effectiveness and accuracy of the model and algorithm proposed in this paper in plasma-induced semiconductor surface state regulation. Through the comparative analysis of multiple sets of experimental and simulation data, it is found that under specific treatment conditions, surface state regulation can significantly improve the photoelectric performance of semiconductor materials, especially in terms of light absorption and carrier separation efficiency.

5. Conclusion

This study systematically explores plasma-induced semiconductor surface state regulation and its influence on the photoelectric properties. By combining experimental verification with simulation analysis, it reveals the key role of surface state regulation in improving the photoelectric performance of semiconductors. The research results show that plasma treatment can effectively change the surface state distribution of semiconductor materials, thereby optimize the carrier recombination path and significantly improve photoelectric conversion efficiency. In the simulation process, based on the precise physical model and algorithm design, the regulation effect of different plasma treatment parameters on the surface state is further verified, and the specific influence of these regulations on the photoelectric properties is quantified. Data analysis shows that under specific processing conditions, the optimization of surface states can enhance light absorption, improve carrier separation efficiency, and ultimately improve overall optoelectronic performance. This study not only proposed a new method for regulating semiconductor surface states through plasma technology but also provided theoretical support and simulation basis for the optimization design of future optoelectronic devices. In general, plasma-induced surface state regulation has significant potential in improving optoelectronic properties, and related algorithms and simulation results have laid the foundation for a deeper understanding of such mechanisms.

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