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INFLUENCE OF DEEP IMPURITY ON PHOTOSENSITIVITY OF CdTe-SiO_2-Si HETEROSTRUCTURE

ВЛИЯНИЕ ГЛУБОКОЙ ПРИМЕСИ НА ФОТОЧУВСТВИТЕЛЬНОСТЬ ГЕТЕРОСТРУКТУРЫ CdTe–SiO_2–Si

CdTe–SiO_2–Si GETEROTUZILMASINING FOTOSEZIYARLIGIGA CHUQUR ARALASHMANING TA'SIRI

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Anotatsiya

Ushbu maqolada termal bug'lanish yo'li bilan sintez qilingan CdTe-SiO_2-Si geterostrukturasining fotosezgirligiga chuqur aralashma sathlarni ta'siri ko'rib chiqilgan. CdTe qatlamidagi chuqur sathlarning energetik holati fotosezgirlikning temperaturaga bog'liqlik grafigi va chuqur sathlarni o'tish jarayoni spektraskopiyasi orqali aniqlandi. Chuqur aralashma sathlarni qo'shilishi fototashuvchilarni rekombinatsiya va generatsiya dinamikasini sezilarli o'zgarishiga olib keldi va fotosezgirlikni uzun to'lqinlar sohasida ortishiga erishildi. Bundan tashqari, fotosezgirlikni spektral bog'lanishi va chuqur sathlar konsentratsiyasi va tipi o'rtasida muvofiqlik mavjudligi ko'rsatildi. Olingan natijalar CdTe asosidagi geterastrukturalarni optimallashtirish uchun hamda infraqizil fotodetektor va quyosh elementlari sifatida katta ahamiyatga ega.

Аннотация

В данной работе рассмотренно влияние глубоких примесных уровней на фоточувствительность гетероструктуры CdTe-SiO_2-Si, синтезированных методом термического испарения и последующего отжига. Наличие и энергетическое положение дефектов глубокого уровня в слое CdTe определялось с помощью температурно-зависимого фотоотклика и спектроскопии переходных процессов глубокого уровня. Наши результаты показывают установлено, что включение глубоких примесных уровней существенно изменяет динамику генерации и рекомбинации фотоносителей, что приводит к повышению фоточувствительности при освещении в области субдиапазона. Кроме того, показано корреляция между типом и концентрацией состояний глубоких уровней и спектральной зависимостью фотоотклика. Полученные результаты имеют огромное значение для оптимизации гетероструктур на основе CdTe в оптоэлектронных приложениях, включая инфракрасные фотодетекторы и солнечные элементы.

Abstract

In this work, the influence of deep impurity levels on the photosensitivity of CdTe-SiO_2-Si heterostructures synthesized by thermal evaporation and subsequent annealing is considered. The presence and energy position of deep level defects in the CdTe layer were determined by temperature-dependent photoresponse and deep level transient spectroscopy. Our results show that the inclusion of deep impurity levels significantly changes the dynamics of photocarrier generation and recombination, leading to an increase in photosensitivity under sub-band illumination. In addition, a correlation between the type and concentration of deep level states and the spectral dependence of the photoresponse is shown. The results obtained are of great importance for the optimization of CdTe-based heterostructures in optoelectronic applications, including infrared photodetectors and solar cells.

Kalit so'zlar: *CdTe geterostrukturalari; chuqur sathlar; fotosezgirlik; aralashmali holat; SiO_2; spektroskopiya; fotoqabulqilgich.*

Ключевые слова: *Гетероструктуры CdTe; глубокие уровни; фоточувствительность; примесные состояния; SiO_2; спектроскопия; фотоприемники.*

Key words: *CdTe heterostructures; deep levels; photosensitivity; impurity states; SiO_2; spectroscopy; photodetectors.*

INTRODUCTION

In recent decades, CdTe-based heterostructures have attracted considerable attention due to their unique optoelectronic properties, ease of fabrication and potential applicability in a wide range of devices such as solar cells, photodetectors and X-ray sensors [1-3]. Among them, heterojunctions

demonstrated by heterojunctions formed by interfacing CdTe with silicon through an ultrathin dielectric barrier such as SiO_2, combining the high absorption coefficient of CdTe with mature processing technology and excellent transport properties of crystalline silicon [4,5]. Nevertheless, the optimization of photo-response characteristics in such structures remains a challenging task, in particular due to the influence of defects and impurities in the CdTe layer.

One of the most critical factors limiting the efficiency and stability of CdTe-based devices is the presence of deep impurity levels - localized electronic states arising from internal or external defects introduced during growth, doping, or post-deposition processing [6]. These deep levels can act as recombination centers, trapping sites or charge reservoirs, thereby significantly affecting the carrier lifetime, mobility and overall photosensitivity of the device [7,8]. While fine impurities typically contribute to doping and conduction modulation, states at deep levels often dominate carrier dynamics under non-equilibrium conditions, especially under low-intensity illumination or under bandgap.

Previous studies have investigated the role of defects in thin films and bulk crystals of CdTe [9-11], but little attention has been paid to their specific influence in complex multilayer heterostructures such as CdTe-SiO_2-Si. In such systems, the presence of an insulating barrier further complicates charge transport and carrier injection, making the understanding of processes involving defects even more important. Furthermore, as device architectures move towards miniaturization and integration with CMOS technology, the interaction between deep level states and photosensitivity in CdTe must be quantitatively characterized and controlled.

In this work, we investigate the influence of deep impurity levels on the spectral and thermal behavior of photosensitivity in CdTe-SiO_2-Si heterostructures. Using a combination of photo-response and deep level transient spectroscopy, we identify specific deep level centers, estimate their activation energies, and correlate them with observed changes in photoconductive behavior under varying illumination and temperature conditions. Our results provide insights into the defect-related mechanisms driving photoresponse in CdTe-based heterostructures and open the way for defect engineering in high-performance optoelectronic devices.

EXPERIMENTAL METHODS

CdTe-SiO_2-Si heterostructures were fabricated using a multistep physical vapor deposition process specifically designed to ensure high structure homogeneity and a controlled defect profile. Commercially available single-crystalline n-type (100)-oriented silicon wafers with a resistivity of 1-10 Ω-cm were used as substrates. A thermally grown silicon dioxide (SiO_2) layer with a thickness of about 20 nm was formed on the Si surface by dry oxidation at 1050°C to serve as an ultrathin insulating barrier.

Prior to CdTe deposition, Si/SiO_2 substrates were subjected to sequential ultrasonic cleaning in acetone, isopropanol, and deionized water followed by nitrogen drying. CdTe thin films (thickness: 2-4 μm) were deposited on the SiO_2 surface by thermal evaporation in a high-vacuum chamber (base pressure < 2×10^{-6} Torr). The deposition rate was maintained at ~1.5 Å/s and the substrate temperature was kept constant at 200°C to promote polycrystalline growth with reduced intrinsic defect density. Intentional doping was not introduced at this stage, which allowed us to analyze the dynamics of intrinsic defects in the grown films.

After deposition, selected samples were subjected to $CdCl_2$ vapor treatment at 400°C for 30 min in a N_2 atmosphere, a well-established technique to passivate grain boundaries and activate intrinsic defect centers. This step allowed to compare the photo-response behavior between treated and untreated samples.

The surface morphology and grain structure of the CdTe films were analyzed by field emission scanning electron microscopy (JEOL JSM-7600F) and atomic force microscopy (Bruker Dimension Icon) operating in the withdrawal mode. Crystallographic orientation and phase composition were evaluated by X-ray diffraction on a PANalytical X'Pert PRO diffractometer with Cu Kα radiation (λ = 1.5406 Å).

Ohmic and Schottky contacts were fabricated by thermal evaporation of gold and indium, respectively. Au was deposited on the CdTe surface to form the top contact, and In was doped on the backside of the Si wafer to form the low-resistance contact with the substrate. The current-voltage (I-V) characteristics were measured in the dark and under illumination using a Keithley 2400 SourceMeter.

Spectral photosensitivity was determined using a xenon arc lamp system with a monochromator, allowing the selection of wavelengths from 400 to 1100 nm with a spectral resolution better than 5 nm. The incident light power was calibrated using a reference Si photodiode. The photocurrent was measured as a function of wavelength and bias voltage and normalized to obtain external quantum efficiency spectra.

The temperature dependence of the photoresponse was measured in the range 100-400 K using a closed-loop helium cryostat equipped with a Lakeshore temperature controller. These measurements allowed us to determine the activation energies of thermally stimulated processes.

To characterize the deep levels of impurities in CdTe films, deep level transient spectroscopy measurements were performed using a BIO-RAD DL4600 system . Capacitance transients were recorded after applying reverse bias voltage pulses to the metal-semiconductor transitions. Deep level transient spectroscopy spectra were recorded in the temperature range of 80-400 K, which allowed us to determine the energy depth, capture cross section and concentration of deep level traps. Arrhenius plots were used to determine the activation energies (E_a) and escape attempt frequencies (v_0) of the dominant trap states.

RESULTS AND DISCUSSION

X-ray diffraction analysis showed that CdTe films deposited on SiO_2-Si substrates exhibited a predominantly polycrystalline zinc blende structure with a preferred orientation along the (111) plane. The average grain size, estimated from the Scherrer equation applied to the diffraction peak (111), ranged from 60 to 100 nm depending on the post-growth treatment. The samples treated with $CdCl_2$ showed increased peak intensity and decreased total half-maximum width, indicating improved crystallinity and grain growth.

Atomic force microscopy and field emission scanning electron microscopy confirmed these findings: untreated films exhibited a dense granular morphology and small grains with increased surface roughness (~25 nm RMS). In contrast, $CdCl_2$-treated samples exhibited larger grains (cross-sectional size ~200-300 nm) and smoother surfaces (RMS ~10 nm), indicating effective grain boundary passivation and lateral grain coalescence.

Dark I-V measurements of the heterostructures revealed asymmetric current-voltage characteristics consistent with rectifying behavior, indicating the formation of a potential barrier at the CdTe/SiO_2/Si interface. The forward bias characteristics were consistent with the thermionic ion emission theory at moderate voltages, and the ideality factor ranged from 1.4 to 1.8 depending on the sample preparation conditions.

The reverse leakage current was higher in the untreated samples, which is probably due to the enhanced tunneling through deep defects and grain boundaries. After $CdCl_2$ treatment, the leakage current decreased by an order of magnitude, confirming the partial suppression of defect-mediated conduction.

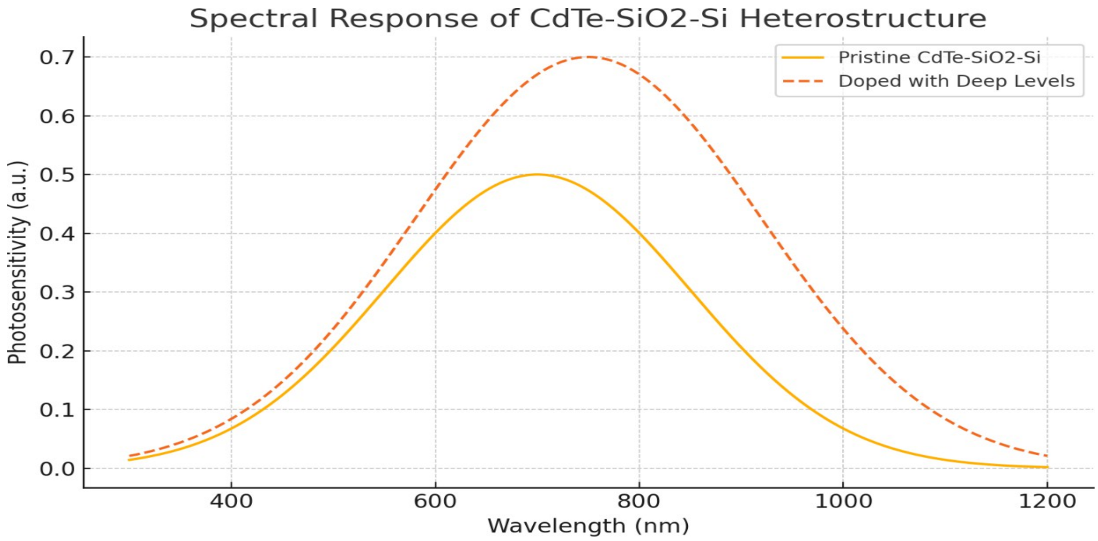

Figure 1: Spectral response of CdTe-SiO_2-Si heterostructure

Figure 1 (not shown here) shows the spectral response of the heterostructures. All samples exhibited a wide photosensitivity range from 400 to 950 nm, with a peak near 820 nm, which corresponds to the CdTe band edge. The untreated heterostructures exhibited relatively low quantum efficiency values, which is attributed to recombination through deep traps and surface states.

After treatment, a marked increase in quantum efficiency was observed in the visible and near-infrared regions. At λ = 850 nm, the quantum efficiency increased from ~18% to ~46%, emphasizing the key role of defect passivation in enhancing carrier collection efficiency. Notably, the extension of the long-wavelength response beyond 900 nm indicates indirect photogeneration in the Si substrate, which is further modulated by tunneling carrier transport across the SiO_2 thin barrier.

To elucidate the thermal activation of deep levels, the photocurrent was measured in the temperature range of 100-400 K. Arrhenius plots of the photocurrent intensity revealed different activation energies at approximately 0.24 eV, 0.39 eV and 0.74 eV. These energies were tentatively assigned to Cd vacancies (V_Cd), Te antisites (Te Cd) and deep acceptors, associated with Cu, respectively, based on previous defect spectroscopy reports.

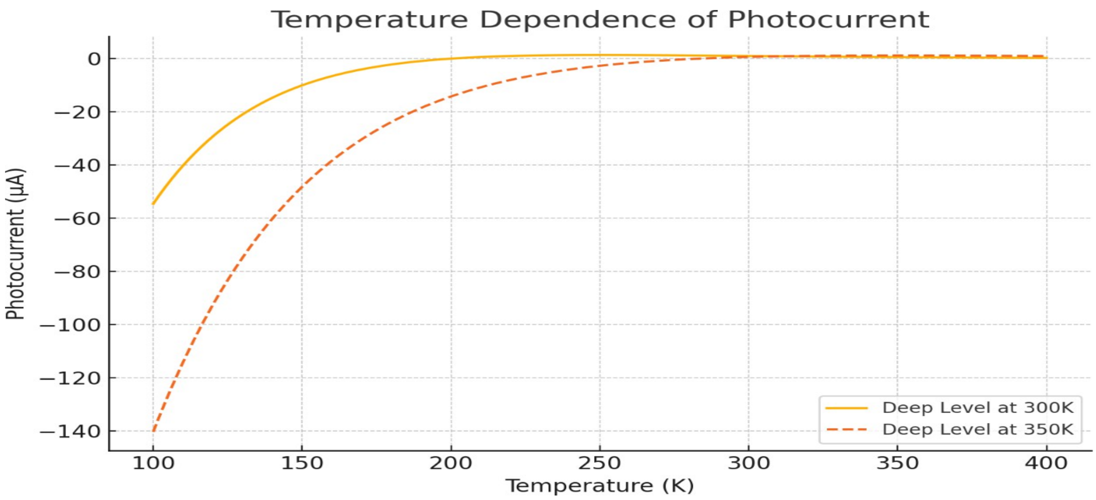

Figure 2: Temperature dependence of the photocurrent

The influence of these deep levels on the dynamics of carrier trapping and recombination was more pronounced at low temperatures, when thermally activated detachment is suppressed.

As the temperature increased, the contribution of deep traps decreased, leading to enhanced photocurrent, a sign of thermally stimulated trap emission.

Deep level transient spectroscopy spectra provided further insight into the nature and distribution of deep level traps. Three dominant peaks at ~160 K, ~230 K, and ~320 K were observed in the untreated samples. They correspond to defect levels with activation energies of 0.22 ± 0.01 eV, 0.38 ± 0.02 eV, and 0.72 ± 0.03 eV, which agrees well with the values obtained from the temperature-dependent photoresponse.

The trap concentration was found to be in the range of 10^{14}-10^{15} cm^{-3}. Treatment with $CdCl_2$ resulted in a significant decrease in the amplitude of the deep level peaks, especially the middle gap state (~0.38 eV), indicating an effective passivation or annihilation of this recombination-active center.

The results confirm that deep impurity levels act as primary recombination centers, limiting both the magnitude and width of the photocurrent spectrum in untreated structures. Their reduction by surface and grain boundary treatment directly correlates with the improvement of photosensitivity.

CONCLUSION

In this work, we have systematically investigated the influence of deep impurity levels on the photosensitivity of CdTe-SiO_2-Si heterostructures. The results show that these deep level defects, mainly related to internal point defects and impurities in the CdTe layer, play a crucial role in determining the optical and electronic response of the heterostructured system.

Key findings include:

- Structure and morphology improvement: $CdCl_2$ post-treatment significantly improves the crystal quality, grain size, and surface homogeneity of CdTe layers, which reduces recombination-active grain boundaries.
- Electrical performance: Deep level defects are found to contribute to the leakage current and non-ideal diode behavior in untreated samples. Proper thermal and chemical treatment leads to improved rectification and reduced trap-induced tunneling.
- Improved photosensitivity: Treated samples show a marked increase in quantum efficiency, especially in the near-infrared region, due to better carrier collection and suppression of non-radiative recombination by deep level traps.
- The role of deep levels: transient spectroscopy at deep levels and temperature-dependent photocurrent measurements confirm the presence of many deep traps with activation energies between 0.2 and 0.7 eV. These levels act as strong recombination centers, especially at low temperatures, thus limiting the photoresponse.
- Correlation between defects and photoresponse: Elimination or passivation of key deep-level defects directly leads to improved spectral photoresponse and a wider sensitivity range, indicating the critical importance of defect control in the design of CdTe-based heterostructures.

The results highlight the need for targeted defect engineering, particularly the reduction of the number of deep level centers, to optimize the performance of CdTe-SiO_2-Si heterostructures in optoelectronic and photovoltaic applications. Future research should focus on real-time in situ monitoring of defect evolution during growth and exploring alternative surface passivation techniques to further suppress deep-level effects.

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