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Detection of carrier information in heterojunctions of nanocrystalline/crystalline Si

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ABSTRACT

Hall effect measurements on heterojunctions of nanocrystalline Si:H (nc-Si:H) film with crystalline Si wafer fabricated by plasma enhanced chemical vapor deposition technique were made as a function of temperature (20–300 K) and magnetic field (0–15 T). Magnetic field-dependent resistivity and Hall data were interpreted with the quantitative mobility spectrum analysis (QMSA) method, which successfully separated the two-dimensional electron gases (2DEGs) at the nc-Si:H/c-Si interface from 3D carriers appearing in the films and substrates. Mobilities and densities of 2DEGs for the specimens were measured. Detail analyses about influences of interface and epitaxial layer quality including doping, film thickness and mean size of nanocrystals on the mobilities and densities of 2DEGs at interfaces were carried out. The important role of the amorphous buffer layer within the junction was identified. Origin of high mobility observed in the prepared films was revealed. Forward and reverse current mechanisms as well as the dependence of breakdown voltages on temperature in the operated nc-Si:H/c-Si heterostructure were elucidated.

1. Introduction

Semiconductor bandgap engineered multilayer structures as promising candidates for infrared detector and high-speed electronic devices usually comprise multiple populations of different carrier species. These carriers may appear in intentional and unintentional doped material layers, surfaces, interfaces and substrates of the heterojunctions (HJs). In the case for presence of diverse carrier species in multilayer units, mixed-conduction effects affect strongly on electronic properties [1]. Several methods have been employed to determine the carrier parameters. Capacitance–voltage electrochemical profiling technique could be adopted to reveal the carrier concentrations in multilayer structures, but invasive nature of the technique can modify 2DEG parameters as a function of each depth while it cannot evaluate the mobilities [2,3]. Time of flight method was used to evaluate the charge carrier drift mobilities in low mobility materials [4]. Single magnetic field Hall effect measurement was used to determine carrier densities, bandgap and impurity activation energies as well as to describe the scattering process involved in the case of single electron, hole conduction, or single band conduction in the semiconductors, but can only extract averaged mobilities and carrier densities. Maximum entropy-mobility spectrum analysis technique as a powerful mathematical approach for investigating the multi-carrier magnetotransport was reported but lacked further experimental evidence [5]. In order to extract detailed information about the transport parameters of these carriers for industrial process control and application, resistivity and Hall effect measurements were performed as functions of magnetic field and temperature in the case of mixed conduction. These variable experimental conditions allow us to simultaneously characterize densities and mobilities for each of the multiple electron and hole species. Further, based on the advantages of multi-carrier fitting method proposed by Gold and Nelson [6], mobility spectrum analysis technique developed by Beck and Anderson [7], and iterative mobility spectrum procedure solved by Dziuba and Gorska [8], Antoszewski et al., Meyer et al., and Hoffman et al. present a quantitative mobility spectrum analysis (QMSA) approach for interpreting magnetic field-dependent resistivity and Hall data from the samples exhibiting mixed conduction [9–11]. This algorithm is fully automated under computer control and requires no decisions on the part of the user. It is thus an eminently suitable and effective mean for deriving accurate and reliable carrier transport parameters in samples such as III–V, II–VI group alloy semiconductors [12–14], and Si-on-insulator (SOI) material [15].

Recently, effective doped nanocrystalline Si:H (nc-Si:H) films have attracted intensive interest in the novel material properties, nanoelectronic and photovoltaic applications [16,17]. Different dimensional carrier species including two-dimensional electronic gases (2DEGs) were observed to exist in nc-Si:H/c-Si heterostructure [18], where the buffer layer was absent. However, an amorphous

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buffer layer is usually incubated between plasma enhanced chemical vapor deposition (PECVD) ultrathin film on c-Si. Because the growth of ultrathin layer needs short time, precursors decomposed from reactive source gas have not enough time to adjust their positions and to match perfectly with the atom array in crystalline substrate. In our recent work, 2DEGs in nc-Si:H/c-Si HJs with a buffer layer was indicated and the correlation between parameters of 2DEG and HJ structures was theoretically simulated [19]. It's reported that 2DEG at semiconductor HJ interface can present technologically advanced application in high electron mobility transistors with high frequency limits and low noise figure of modulation doped field-effect transistors [20,21], thus further inspirits us to probe the origination and properties of 2DEGs in nc-Si:H/c-Si HJs, which yield a new way to produce HJ with salient advantages of 2DEG. In present work, in order to explore formation and characteristics of 2DEGs as well as conduction mechanisms in the prepared nc-Si:H/c-Si HJs, a series of different phosphorus doped nc-Si:H films and another series nc-Si:H films with different hydrogen (H_2) diluted silane (SiH_4) at fixed doping level were deposited by PECVD method on an identical batch medium doped (p)c-Si substrates. After structural check and electronic measurements, 2DEGs at interfaces were indicated while the effect of interface and epitaxial layer quality including doping, film thickness and mean sizes of nanocrystals on the mobilities and densities of 2DEGs were analyzed. Transport behaviors in the formed HJ were also elucidated.

2. Experimental details

The nc-Si:H/c-Si units were produced with a planer process. One identical batch single facet polished p-type (111) c-Si wafers with around 100 μm thickness and average resistivity of ~10 Ω cm ($N_A \sim 10^{15}$ cm^{-3}) were utilized. Film growth was operated in a capacitively coupled radio frequency (RF) of 13.56 MHz powered PECVD system assisted with direct current (DC) bias stimulation. SiH_4 and phosphine (PH_3) as well as H_2 were mixed up as reactant gas. The first (F) series of nc-Si:H/c-Si HJs were fabricated at fixed diluting ratio $SiH_4/H_2 = 1.00$ vol% (volume percentage) while varying doping ratio PH_3/SiH_4 vol% and film thickness, the parameters are presented in Table 1. Additionally, the second (S) series of HJs were deposited at fixed doping ratio $PH_3/SiH_4 = 0.8$ vol% while changing diluting ratio SiH_4/H_2 vol% and film thickness individually, the parameters are exhibited in Table 2. The film thickness was strictly controlled by adjusting the film growing time separately. Diluting ratio and doping ratio adopted herein were ever employed to fabricate successfully high quality specimens in elsewhere [16,17]. Other process parameters were set as follows: substrate temperature of 373 ± 1 K, RF power density of 0.60 ± 0.05 W/cm^2, reactant gas pressure of 100 ± 5 Pa and DC voltage of −200 ± 2 V applied to the substrate.

A high resolution transmission electronic microscope (HRTEM) photo for a cross-section of nc-Si:H/c-Si HJ of specimen S34 (deposited with doping ratio of 0.8 vol% and diluting ratio of 1.2 vol%) was taken by a JEM-2010 instrument operating with voltage of 100 kV and resolution of 0.19 nm, as depicted in Fig. 1.

Table 1
The primary parameters of the first (F) series of nc-Si:H/c-Si HJs deposited at fixed diluting ratio while varied doping ratio and film thickness respectively. The value of about 40, 60 and 80 nm stands for film thickness.

Serial number (Fmn) m:1 ~ 3; n:1 ~ 4	Diluting ratio (SiH_4/H_2 vol%)	Doping ratio (PH_3/SiH_4 vol%)			
		0.2	0.4	0.8	1.6
F1n	1.0	41 nm	40 nm	41 nm	42 nm
F2n		59 nm	62 nm	61 nm	60 nm
F3n		80 nm	79 nm	82 nm	81 nm

Table 2
The main parameters of the second (S) series of nc-Si:H/c-Si HJs fabricated at fixed doping ratio while varied diluting ratio and film thickness respectively. The value of about 40, 60 and 80 nm stands for film thickness. In last row, 2.2, 3.3, 4.3 and 5.5 nm stand for mean size of nanocrystallite for the films deposited with diluting ratio of 0.6, 0.8, 1.0, 1.2 vol% respectively.

Serial number (Smn) m:1 ~ 3; n:1 ~ 4	Doping ratio (PH_3/SiH_4 vol%)	Diluting ratio (SiH_4/H_2 vol%)			
		0.6	0.8	1.0	1.2
S1n	0.8	40 nm	41 nm	41 nm	39 nm
S2n		60 nm	59 nm	61 nm	61 nm
S3n		81/2.2 nm	80/3.3 nm	82/4.3 nm	82/5.5 nm

The average size d_{Raman} of nanocrystalline Si was estimated according to HRTEM technique while the film thickness was measured by TEM.

In order to check whether 2DEGs occur in the produced HJs, the measured samples for Hall effect experiments were prepared with van der Pauw configuration, i.e., the wafers were sliced into square pieces of 2 × 2 mm^2, then Ohmic contact electrodes of Au/Ge alloy with about 0.2 mm^2 area were deposited by a ZZSX-800A type electron beam evaporation apparatus (made by Beijing instrument factory in China) on the four corners of the square piece of nc-Si:H film through a grid. Hall effect measurements were made by an Oxford Instruments superconductive magnet at 13 temperature step across a range of 20–300 K and at 30 magnetic field intensity step across a range from 0 to 15 T. The experimental results are presented in Fig. 2.

Au/Cr and Au/Ge alloys as Ohmic contact electrodes were prepared by the foregoing electron-beam evaporation instrument on both sides of substrate and nc-Si:H film respectively, Subsequently, the units of electrode/nc-Si:H/c-Si/electrode were sealed in ceramic shells with metal contact pads to perform current–voltage (I–V) measurement. Within the temperature range of 20–300 K, I–V data of these studied units were recorded by a computer-controlled system (including a KEITHLEY 6514 electrometer and a KEITHLEY 2410 sourcemeter). The I–V experimental data for sample S34 are offered in Fig. 3.

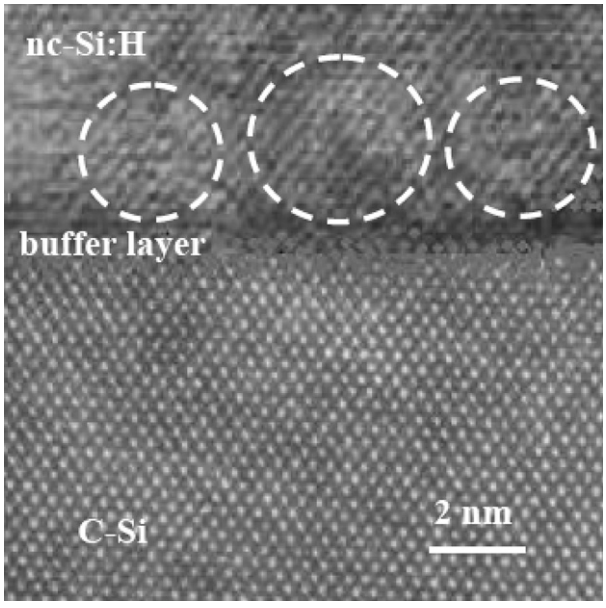

Fig. 1. A HRTEM photo of cross-section of nc-Si:H/c-i HJ (specimen S34, deposited with diluting ratio 0.6 vol% and doping ratio 1.2 vol% respectively). A buffer layer with around 1–2 nm thickness is incubated on the c-Si substrate.