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Electrical and Photoluminescence Characteristics of Nanocrystalline Silicon-Oxygen Superlattice for Silicon on Insulator Application

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Abstract - Electrical forming dependent current-voltage (I-V) and numerically derived differential conductance (dI/dV) characteristics have been presented in the multi-layer nano-crystalline silicon/oxygen (nc-Si/O) superlattice. Distinct staircase-like features, indicating the presence of resonant tunnel barriers, are clearly observed in the dc I-V characteristics. Also, all samples showed a continuous change in current and zero conductivity around 0V corresponding to the Coulomb blockade in the calculated dI/dV-V curve. Also, Raman scattering measurement showed the presence of a nano-crystalline Si structure. This result becomes a step in the right direction for the fabrication of silicon-based optoelectronic and quantum devices as well as for the replacement of silicon-on-insulator (SOI) in high speed and low power silicon MOSFET devices of the future.

Keywords : current-voltage (I-V), differential conductance-voltage (dI/dV-V), photoluminescence (PL)

1. Introduction

Silicon is by far the most widely used semiconductor and its properties are well known and understood. However, lacking a direct fundamental bandgap, it does not play an important role in photonic devices. Since the discovery of visible photoluminescence (PL) from porous silicon [1], it seems that a process which is compatible with the silicon processing industry is finally at hand for photonic devices.

R. Tsu suggested superlattices [2] and quantum wells [3] with L. Esaki in 1970 and 1973, respectively. After that, the use of nanoscale silicon particles imbedded in an oxide matrix was introduced [4,5] for possible silicon quantum devices operated at room temperature. A diode structure with annealing and oxidation of a thin amorphous silicon layer sandwiched between oxide layers, followed by a proper electrical forming process [6], was chosen for this work. It is noted that electrical forming is essential for the minimization of possible breakdowns with high electric fields [7], as well as serving as a selection of particle sizes. The evidences of resonant tunneling via nanoscale silicon imbedded in an oxide matrix are confirmed from those works. Recently, R. Tsu and coworkers reported a new type of superlattice formed by replacing the heterojunction between adjacent semiconductor layers by a monolayer of adsorbed species such as oxygen atoms, and CO molecules [8-11].

In this work, we have studied electronic transport and photoluminescence characteristics as functions of annealing conditions in the multilayer nanocrystalline silicon/oxygen (nc-Si/O) superlattice formed by a molecular beam epitaxy (MBE) system, to explore several strategies towards developing silicon-based optoelectronic devices. The electrical forming dependent I-V and dI/dV characteristics have been presented. Also, Raman scattering measurement was performed to investigate photoluminescence characteristics as a function of annealing conditions. Consequently, the experimental results of our multilayer device showed stable photoluminescence and good insulating behavior with high breakdown voltage. This is very useful for Si-based optoelectronic devices, and can be readily integrated with conventional silicon ultra large scale itegrated circuits (ULSI) processing for SOI application.

2. Experiments

nc-Si/O superlattices were prepared in an ultra high vacuum (UHV) molecular beam epitaxial (MBE) system with a growth chamber base pressure of $\sim 10^{-10}$ Torr. Antimony (Sb) doped buffer silicon of 200 nm was deposited by electron beam (e-beam) onto a single crystalline n-type (100), $\rho \approx 0.01$ - 0.1 Ω·cm silicon substrate. Then the samples were prepared at various temperatures: room temperature (RT), 300 °C and 550 °C, all with a silicon layer thickness of 1.2 nm. After oxygen exposure was

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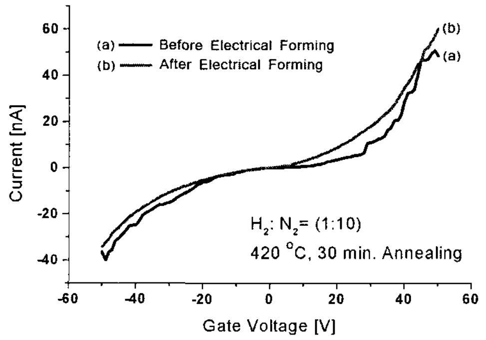
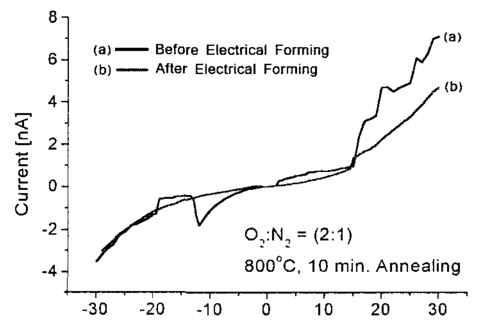
carried out at room temperature for 20 minutes, typically 1.2 nm of silicon was deposited. This process was repeated a number of times. A total of nine period Si/O superlattices were grown, and the silicon deposition rate was kept at 0.5 Å / sec. In order to investigate the electronic and optical characteristics as a function of annealing conditions, the first sample was annealed in H_2 + N_2 (1:10) at 420 °C for 10, 20, and 30 minutes, respectively. The second sample was annealed in O_2 + N_2 (2:1) at 800 °C for 10 min. Hydrogen gas was used for the passivation of dangling bond defects, while nitrogen served as a forming gas. The dc I-V measurements were performed with a Keithley 236 I-V system. The spectrum of PL was obtained with a U-1000 Yvon-Jobin monochrometer and detected with a R-943 Hamamatsu PMT. The 457.9 nm line of the argon laser was used for the PL spectrum.

3. Results and discussion



(a) °C, 30 minutes hydrogen annealed samples



(b) 800°C, 10 minutes oxygen annealed samples

Fig. 1 The staircase-like current-voltage characteristics as a function of different annealing conditions; (a) 420°C, 30 minutes hydrogen annealed samples, (b) 800°C, 10 minutes oxygen annealed samples.

Fig. 1 compares the I-V characteristics of (a) 420°C, 30 minutes hydrogen-annealed and (b) 800°C, 10 minutes oxygen-annealed samples before and after the electrical forming process. During the first measurement, as the voltage increases, the current showed staircase-like features due to resonant tunneling and quantum confinements. However, after the second measurement, the steps disappeared and the current was exponentially increased. This is due to the thermally activated recrystallization of nc-Si and removal of oxygen precipitates around the nc-Si during the subsequent measurements, which can perhaps be explained by an electro-thermal forming cycle [6] between the two measurements. Also, a similar result was observed in the reverse region. Steps at negative bias represent the incremental charging of nc-Si and those at positive bias represent the decremental charging. That is, the charge was trapped within the device.

Up to a bias of 30 V, there is no sign of breakdown, which indicates that this multilayer Si/O superlattice barrier can be used in the isolation of Si devices. However, the low-voltage isolation is not sufficient for implementation as a substitute for SOI. Increasing the number of periods may offer the needed requirements. This thick barrier may be useful as an epitaxial insulation gate for field effect transistors (FETs). The rationale is that it should be possible to fabricate FETs on top of each other, moving one step closer to the ultimate goal of a three-dimensional integrated circuit (3D-IC)[10].

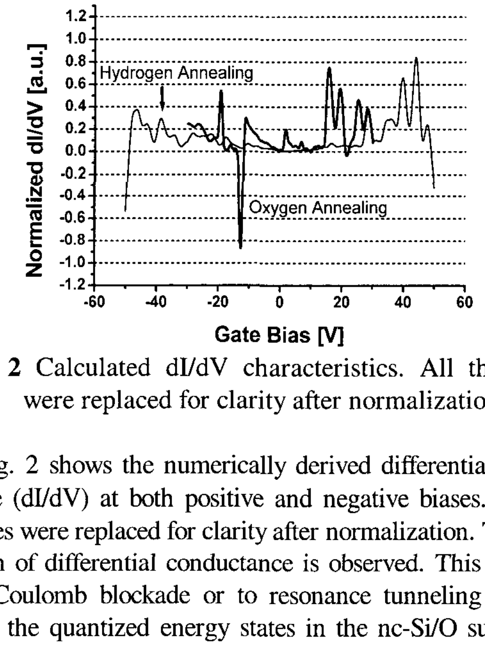


Fig. 2 Calculated dI/dV characteristics. All the curves were replaced for clarity after normalization.

Fig. 2 shows the numerically derived differential conductance (dI/dV) at both positive and negative biases. The two curves were replaced for clarity after normalization. The oscillation of differential conductance is observed. This is due to the Coulomb blockade or to resonance tunneling resulting from the quantized energy states in the nc-Si/O superlattice structure. The peaks in the normalized dI/dV curves are oscillations between two conducting states (strongly conducting level and weakly conducting level) in the Si-O superlattice device. The oscillation may be due to trapping centers close to the resonant energy levels. Successive charge trapping and detrapping result in continuous decrease and increase in the conduction process, respectively. In the Si/O superlattice device, quantum confinement could possibly occur if the nanocrystallites were surrounded and confined by an adsorbed oxygen layer. Also, it is important to point out the negative differential conductance (NDC) characteristics. There is negative conductance, which is probably due to hot carrier injection into the silicon capping region and the silicon buffer region undergoing avalanche multiplications. Resonant tunneling via some in-advertent isolated defects are probably responsible for the initiation of the process. The detail of the dI/dV characteristics is really far more complex. A simple explanation based on resonant tunneling without a model including trapping mechanisms cannot offer a satisfactory understanding at this point. That is, the appearance of jumps and negative conductance indicates the presence of electrically active defects and traps, which may be reduced by further investigation involving the passivation and optimization of parameters, such as the thickness of the thin silicon as well as the oxygen exposure [10].

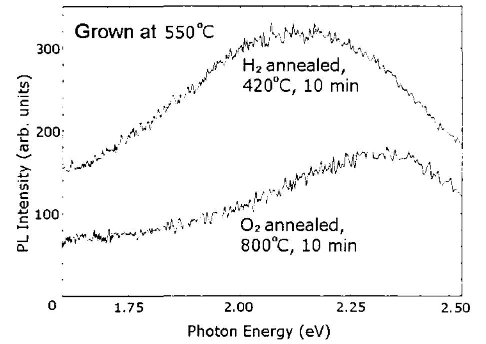


Fig. 3 Photoluminescence spectra of a nine period nc-Si/O superlattice grown at 550 °C, with 1.2 nm thickness of each Si layer, annealed in hydrogen and oxygen.

Fig. 3 shows the photoluminescence spectrum of a sample grown at 550 °C, with a silicon layer thickness of 1.2 nm [11]. The sample was annealed in hydrogen at 420 °C for 10 minutes, and in oxygen at 800 °C for 10 minutes, respectively. The photoluminescence of the hydrogen-annealed sample was considerably stronger, which indicates a better quality of passivation. It is known that although oxygen can also provide some passivation, hydrogen passivation is essential for efficient luminescence [12]. Figure 3 also shows that the photoluminescence spectrum of the oxygen-annealed sample is blue shifted by approximately 250 meV, indicating a further reduction in the particle size as a result of oxygen annealing. After establishing the importance of hydrogen annealing for efficient luminescence, we proceeded to examine the role of the crystallinity of the silicon cluster in the luminescence.

Fig. 4 shows the PL spectra for three samples with a silicon layer thickness of 1.2 nm and deposited at three temperatures: room temperature (RT), 300 °C and 550 °C [11]. All samples were annealed in hydrogen at 420 °C for 20 minutes. The crystallization of such thin layers is restricted by the proximity of the adjacent adsorbed oxygen gas molecules. It is noted that at room temperature deposition and 420°C hydrogen annealing, the silicon remains in a primarily amorphous state. Raman scattering shows only partial crystallization. Therefore, the photoluminescence spectra is expected to be blue shifted. In fact, our PL peak at 2.3eV photon energy compares closely to that reported in reference [13]. The photoluminescence from the sample deposited at 550 °C is red shifted. This red-shift can be explained in terms of increased crystallization and a subsequent increase in the cluster size. Raman scattering shows significant crystallization for this sample. In addition, note that the photoluminescence intensity for the 550 °C grown sample is considerably higher, indicating that crystallization leads to stronger luminescence. The photoluminescence spectrum of the sample grown at 300 °C appears to be intermediate, both in photon energy peak and in photoluminescence intensity. The above analysis from Fig. 3 and Fig. 4 indicates that quantum confinement gives rise to a greater blue-shift for smaller crystallites. That is, the blue-shift in the PL peak of the sample with oxygen anneal, compared to the sample with hydrogen anneal, is due to a contribution from smaller crystallites.

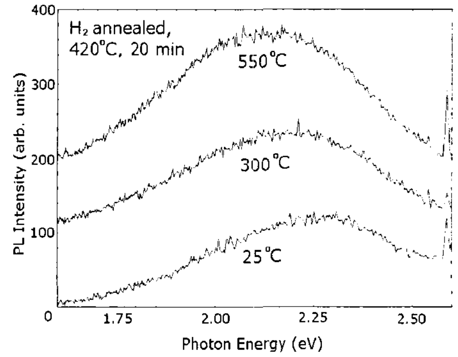


Fig. 4 Photoluminescence spectra of three nine period nc-Si/O superlattice samples with 1.2 nm thickness of each Si layer, grown at 550 °C, 300 °C, and 25 °C, respectively. All samples were annealed in hydrogen and nitrogen, at 420 °C for 20 minutes.

The energy band diagram of the device, under reverse bias, is shown in Fig. 5 taken from reference [14]. The native oxide forms a thin oxide barrier as shown.

Under reverse bias, electrons from the metal side are injected into the superlattice through the thin oxide. These electrons remain hot and undergo avalanche multiplication, generating new electron-hole pairs into the silicon. While the generated electrons slide down the energy slope, the holes move up the energy incline and eventually are trapped in the superlattice, where they radiatively recombine with the plentiful electrons from the conduction band of the n-type material. It is important to mention that holes can tunnel through the thin oxide into the metal. Therefore, under increased levels of reverse bias, our device is driven into deep depletion, preventing the formation of inversion. We should also mention that electrons are abundant in our n-type silicon material. However, since under normal circumstances holes are not plentiful in an n-type material, operation of our device relies on the avalanche process to generate the holes necessary for recombination. Electrons injected into the depletion region of our device are accelerated under the effect of the strong electric field, thereby increasing their energy with respect to the bottom of the conduction band. As the electrons move inside the material, they constantly collide with the lattice, losing some of their energy. Electrons having an energy larger than the energy gap, have the opportunity during this process to generate an electron-hole pair by impact ionization. As the process is repeated, more and more electron-hole pairs can be generated. Presumably, this is the process by which the holes necessary for recombination and therefore light emission are generated within the device.

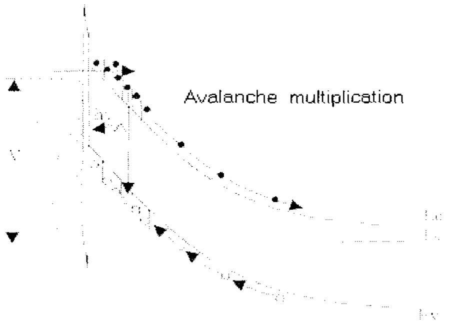


Fig. 5 Energy band diagram of the Si/O superlattice device under reverse bias. Electrons undergo avalanche multiplication providing holes for radiative recombination.

4. Conclusions

The staircase-like I-V characteristics and oscillation of the differential conductance of silicon/oxygen superlattice formed by a molecular beam epitaxy system (MBE) have been presented. Distinct staircase-like features, indicating the presence of resonant tunnel barriers, are observed in the dc I-V characteristics. Also, coulomb blockade oscillation was obtained in a numerically derived dI/dV-V curve. Raman scattering measurement showed the presence of a nanocrystalline Si structure. The blue-shift was observed in the PL peak of the oxygen-annealed sample, compared to the hydrogen-annealed sample, which is due to a contribution from smaller crystallites. Consequently, the experimental results showed stable photoluminescence and good insulating behavior with high breakdown voltage. Thus, the Si/O superlattice can serve as a barrier as well as isolation for Si devices.

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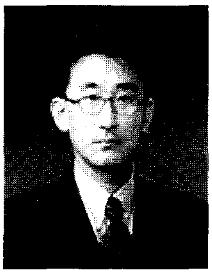

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