TAILORING OF Si NANOSTRUCTURES EMBEDDED INTO EPITAXIAL OXIDES FOR VARIOUS APPLICATIONS

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Introduction

Successful integration of low-dimensional crystalline silicon into insulator barrier layers could open the way for a variety of novel applications ranging from insulator/silicon heterostructures for nanoelectronic application in future quantum-effect devices to the next generation of solar cells.
Double-barrier structures comprising epitaxial insulator as barriers and Si as quantum-well are interesting because of its applicability for tunneling devices [1]. Furthermore, quantum confinement of charge particles within nanostructured materials could lead to a large number of new phenomena, which could never been realized in normal bulk materials. In conventional bulk semiconductors, for example, a single electron-hole pair is generated by single photon absorption. However, if we reduce the size of Si clusters down to the quantum regime, higher energy photons can produce multiple charge carriers by a process known as impact ionization. Such effect could pave the way for new generation of solar cells with ultrahigh efficiencies [2]. Furthermore, Si nanoclusters (NCs) embedded into dielectric insulator could be one of the potential contenders for non-volatile memory device applications [3].
Here we will report on the preparation and properties of multi-dimensional Si nanostructures buried into the dielectric rare-earth oxide material (Gd_2O_3), which crystallizes in the cubic bixbyite (Mn_2O_3) structure. Gadolinium oxide is a suitable insulator with a large band gap of about 6 eV, nearly symmetrical band offset to Si at the Gd_2O_3/Si interface as well as a low lattice mismatch of about 0.5% to Si [4], respectively. The electrical properties make Gd_2O_3 interesting also for integration into conventional (MOS) Si devices [5].

Experimental

Gd_2O_3/Si/Gd_2O_3 stacks were fabricated on Si(111) and Si(001) substrates under ultra-high vacuum conditions using molecular beam epitaxy (MBE) technique. Silicon and granular stoichiometric Gd_2O_3 were evaporated by electron-beam heating.
The physical properties of structures containing Si-NCs and quantum wells were investigated by x-ray diffraction, photoluminescence (PL) spectroscopy, capacitance-voltage (C-V) and current-voltage (I-V) measurements.

Results and Discussion

Fig.1 shows various Si nanostructures embedded into epitaxial Gd_2O_3 on Si(111) substrates. The structures were obtained by a novel approach developed recently [6]. Thereby, the shape, distribution and number of Si-NCs were controlled by modifying the growth kinetics during MBE.

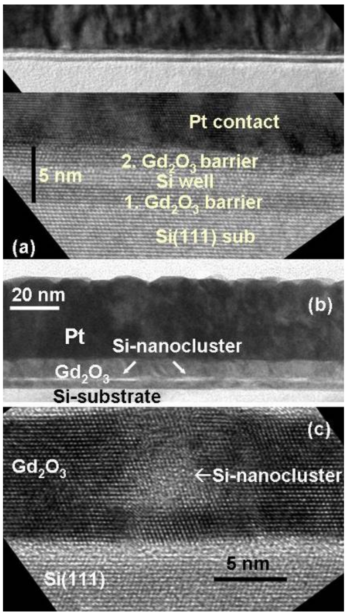
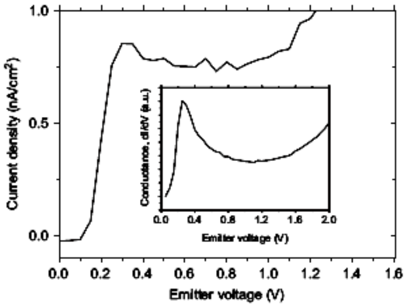


Fig.1 Cross-sectional TEM lattice images of Si nanostructures embedded into single-crystalline Gd_2O_3 on Si(111) substrates, (a) Si quantum well, (b) and (c) Si nanocluster.



I-V characteristic for a double-barrier structure on Si(111).

As demonstrated in Fig.2, I-V characteristics obtained for structures containing Si-quantum wells exhibit negative differential resistance, making them an attractive candidate for resonant tunneling devices.

Fig. 3 presents C-V measurements for MOS capacitors containing Si-NCs on n-type Si(111) and Si(001). Electron injection from the substrate results in a clockwise hysteresis due to a significant shift of the flat band voltage under charging/discharging conditions (±5V for Si(111) and ±7V for Si(001)) indicating an excellent charge storage behavior. The observed flat band voltage shift of around 1 V corresponds to a storage rate of nearly two electrons per Si nanocluster.

Fig.4(a) and (b) show PL spectra of samples containing Si-NCs with sizes of about 4.5 and 3.5 nm, respectively. Blue shift in the peak position with respect to bulk Si for samples with smaller dots is consistent with quantum confinement effect behavior. The peak at ΔE = 0.67 eV in 4(b) is due to the presence of localized surface states.

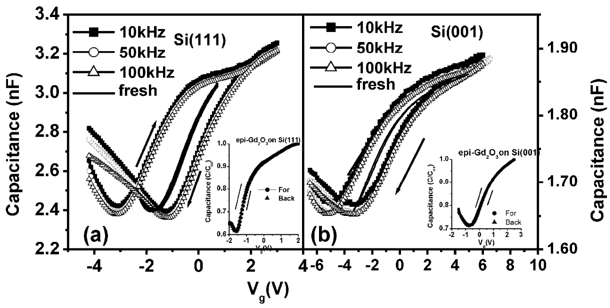


Fig.3 C-V characteristics of Pt/Gd_2O_3/Si MOS capacitors with embedded Si-NCs grown on (a) Si(111) and (b) Si(001). The solid line displays the hysteresis loop of fresh device demonstrating that the clusters are not charged. (The insets show the hysteresis behavior of Gd_2O_3 layers without Si-NCs.)

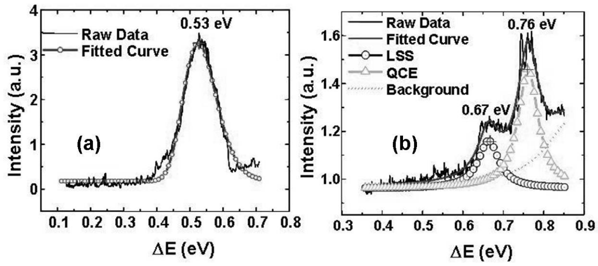


Fig.4 Photoluminescence spectra of samples with (a) 4.5 nm and (b) 3.5 nm Si-NCs together with fitted and simulated data.

Conclusions

Heterostructures containing Si nanostructures buried in epitaxial Gd_2O_3 were investigated by various techniques. The structures were prepared on Si substrates by a novel approach based on a modified epitaxy technique. The obtained properties for this unique kind of heterostructure indicate numerous possible applications in different fields like electronics, optics and solar cells.

References

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