Static dielectric constant of SiO_2 embedded with silicon nanocrystals

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ABSTRACT

In this work, the static dielectric constant of silicon nanocrystal (nc-Si) embedded in SiO_2 matrix has been determined from the Maxwell-Garnett effective medium approximation (EMA) and the stopping range of ions in matter simulation. From the capacitance-voltage measurements, slight increment in the total capacitance at strong accumulation is observed, indicating that the dielectric constant of the SiO_2 film embedded with nc-Si is no longer a constant value of 3.9. The mean size of nc-Si as determined from the TEM measurement corresponds to a dielectric constant of ~9.6, being consistent with other theoretical predictions. The suppression of this value is due to the surface effect. The information obtained from this study is useful to future modeling of nc-Si based memory devices.

Keywords: silicon nanocrystal, dielectric constant, silicon dioxide

1 INTRODUCTION

Utilizing nanocrystals or quantum dots embedded in SiO_2 matrix as charge storage elements has drawn many researchers' interest in the field of optical properties [1], memory characteristics [2-3] as well as current transport [4]. One of the promising techniques to incorporate nc-Si into SiO_2 is Si ion implantation followed by high temperature annealing. With this technique the fabrication is fully compatible with the mainstream CMOS process and the distribution of nc-Si in the gate oxide can be easily controlled. When the nc-Si is embedded in the SiO_2 film, the dielectric constant of the film will be different from that of pure SiO_2 film. Therefore, for flash memory devices with the nc-Si embedded in the gate oxide, the inclusion of the nc-Si will definitely affect the gate capacitance. In despite of the importance in design and modeling of the memory devices, a quantitative study on the influence of nc-Si on the gate capacitance is still lacking. In this work, we present an approach to calculate the static dielectric constant of isolated nc-Si embedded in the SiO_2 matrix. The nc-Si is implanted into the SiO_2 and subsequently annealed at high temperature. Moreover, the influence of different nc-Si distributions in the SiO_2 on the total gate capacitance will also be discussed. Our approach is proven to be reliable by comparison with the results of other theoretical calculations.

2 APPROACH

It is observed that the total gate capacitance of a SiO_2 embedded with nc-Si is slightly higher than that of a pure SiO_2 film. This shows that the introduction of nc-Si inside the SiO_2 will definitely change the properties of the material. Besides, the nc-Si is an isolated nanoscale structure with a size of less than 5 nm embedded in the SiO_2 matrix, its physical properties should be different from that of bulk crystalline Si. Other than the increase in the capacitance, Fig. 1 also shows that the inclusion of the nc-Si leads to a flatband voltage shift. The shift is due to the charge trapping in the nc-Si during the C-V measurement and the difference in the work function between the nc-Si and the SiO_2.

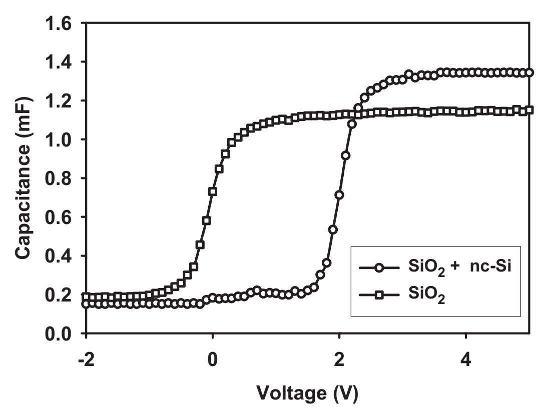


Figure 1: Capacitance-Voltage (C-V) measurements on the samples with and without nc-Si.

The depth profile of the implanted nc-Si in the SiO_2 film can be obtained from the Secondary Ion Mass Spectroscopy (SIMS) measurements or the stopping and range of ions in matter (SRIM) simulation. Both of these methods can produce quite an accurate nc-Si profile. When this profile is obtained, the volume fraction of the nc-Si in the SiO_2 can be calculated based on below equation

$$v(x) = \frac{QI(x)}{N_{Si}\int_0^{l_{\max}} I(x)dx} \qquad (1)$$

where Q is the dosage of implanted Si ions, d_{max} is the maximum depth of the Si implantation profile, N_{Si} is the silicon density and $I(x)$ is the Si SRIM / SIMS intensity.

To model the effective dielectric constant of the thin film embedded with nc-Si, the SiO_2 with thickness of T_{oxide} can be divided into m sub-layers. Thus, each sub-layer has an equivalent thickness of T_{oxide}/m, as shown in Fig. 2a. The effective dielectric constant, ε_i (i = 1,2,…,m) for each of the i^{th} sub-layer can be calculated with the Maxwell-Garnett effective medium approximation (EMA), as given by

$$\frac{\varepsilon_i - \varepsilon_{SiO2}}{\varepsilon_i + 2\varepsilon_{SiO2}} = v_i \frac{\varepsilon_{nc-Si} - \varepsilon_{SiO2}}{\varepsilon_{nc-Si} + 2\varepsilon_{SiO2}} \qquad (2)$$

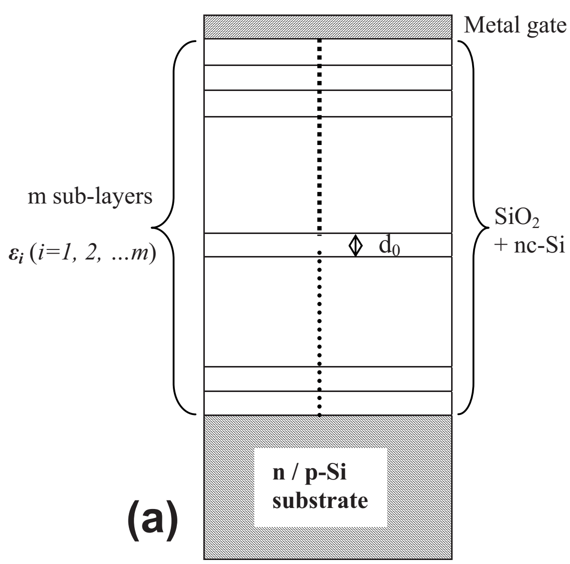
where v_i (i = 1,2,…, m) is the volume fraction of the nc-Si in the i^{th} sub-layer, ε_{nc-Si} is the static dielectric constant of nc-Si, and ε_{SiO2} is the dielectric constant of pure SiO_2. The MOS capacitance (C) per unit area can be expressed as

$$\frac{1}{C} = \sum_{i=1}^{m} \left[\frac{m\varepsilon_i \varepsilon_0}{T_{oxide}}\right]^{-1} \qquad (3)$$

where ε_0 is the permittivity in vacuum.

If the Si-ions is only implanted into portion of the SiO_2, there will be a layer of SiO_2 without nc-Si. Eq. (3) is no longer valid. The modeling of such structure is shown in Fig. 2b and the total MOS capacitance of this structure can be expressed as

$$\frac{1}{C} = \sum_{i=1}^{m} \left[\frac{m\varepsilon_i \varepsilon_0}{d_{max}}\right]^{-1} + \left[\frac{3.9 \times \varepsilon_0}{T_{oxide} - d_{max}}\right]^{-1} \qquad (4)$$



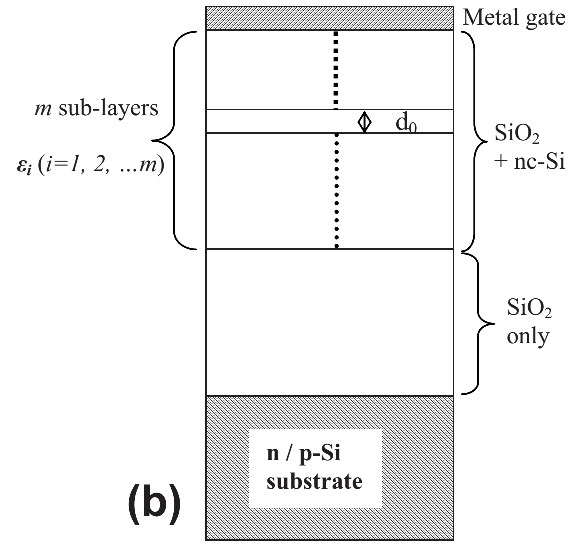


Figure 2: Model used for the EMA calculation for a full distribution (a) and partial distribution (b) of nc-Si in the SiO_2 film.

3 RESULTS AND DISCUSSIONS

For the sample shown in Fig. 1, Eq. (3) is used to calculate the total MOS capacitance due to the full nc-Si distribution in the entire SiO_2 matrix. Fig. 3 shows the calculated MOS capacitance as a function of ε_{nc-Si} which varies from 3.9 (dielectric constant of SiO_2) to 11.9 (dielectric constant of bulk crystalline silicon). The measured capacitance is plotted together in Fig. 3. From the curve of the capacitance versus the ε_{nc-Si} shown in Fig. 3, we can find the value of ε_{nc-Si} corresponding to the measured MOS capacitance of the structure with the nc-Si distributed in the oxide. The value obtained is ~9.6, and it is actually the dielectric constant of the nc-Si embedded in the oxide. This value is significantly smaller than that of bulk crystalline silicon but larger than that of a SiO_2.

To verify the accuracy of our approach, the obtained static dielectric constant is compared with other theoretical calculations. The screening dielectric constant of nc-Si can be theoretically calculated with the formula below [5]:

$$\varepsilon_{nc-Si}(D) = 1 + \frac{\varepsilon_b - 1}{1 + \left(\frac{1.38}{D}\right)^{1.37}} \qquad (4)$$

where ε_b is the dielectric constant of bulk crystalline silicon and D is the diameter of nc-Si in the unit of nm. By fitting the $\varepsilon_{nc\text{-}Si}$ as 9.6, the diameter of the nc-Si is ~4.3 nm. This dielectric constant of nc-Si is consistent with others theoretical calculations for the nc-Si with a mean size of ~4.5 nm.

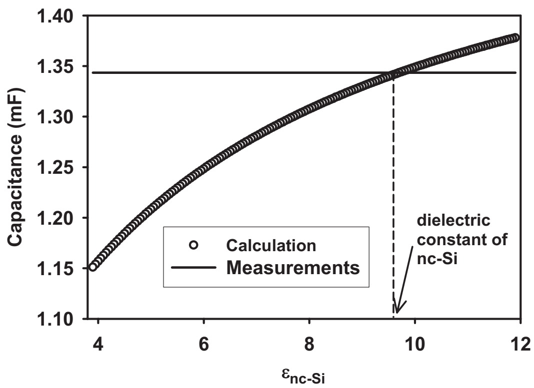


Figure 3: Determination of dielectric constant of nc-Si based on the comparison of the calculation with the experiment.

Fig. 4 shows the high resolution transmission electron microscopy (TEM) measurements for the sample with nc-Si. The size of the nc-Si is ~4.4 nm. By setting the D equals to 4.4 nm, the static dielectric constant of nc-Si based on Eq. (4) is found to be 9.6, again being consistent with the measurements as shown in Fig. 3.

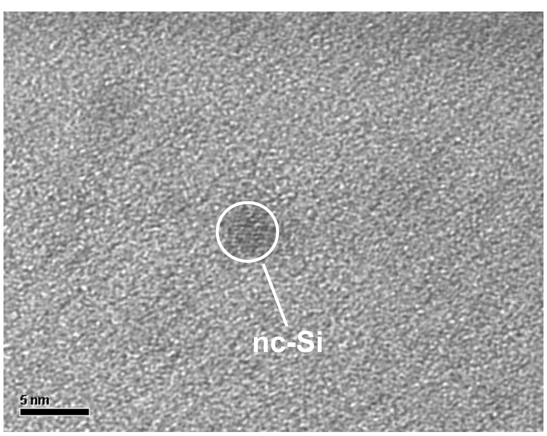


Figure 4: Cross section TEM measurements of the sample.

In order to further verify the accuracy of our approach, the influence of different nc-Si distributions on the total MOS capacitance is being studied. Figure 5 shows the influence of implantation energy on the MOS capacitance. The capacitance is calculated at various implantation energies ranging from 1 keV to 11 keV and the gate oxide thickness of 30 nm. According to the SRIM output, for a 30 nm gate oxide, the partial distribution as shown in Fig. 2a corresponds to implantation energies lower than 7 keV, while the full distribution as shown in Fig 2b is achieved with implantation energies higher than 7 keV. The overall effect of the implantation energy on the MOS capacitance for the partial distribution is that the MOS capacitance first decreases as the implantation energy increases and then it increases slowly when the energy is larger than ~2 keV, as shown in Fig. 5. For the full distribution, when the implantation energy is larger than 7 keV, some of the Si ions are implanted into the Si substrate. Therefore, as the implantation energy increases, the effective dielectric constant ε_i decreases as a result of the decreasing nc-Si volume fraction (v_i). The experimental measured capacitance is plotted together in Fig. 5. Good agreement between the measured and the simulation capacitance proves that our approach is valid for different distribution of nc-Si in SiO_2. Besides, the simulation of the capacitance based on the dielectric constant of crystalline bulk Si (11.9) is also plotted together. This graph clearly shows that the nc-Si embedded inside the SiO_2 matrix should not be the same as the bulk Si.

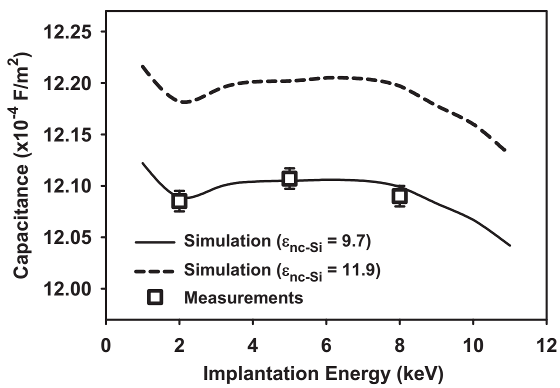


Figure 5: Influence of Si^+ implantation energy on the MOS capacitance.

The influence of SiO_2 thickness on the MOS capacitance with and without nc-Si is shown in Fig. 6. The $\varepsilon_{nc\text{-}Si}$ is fixed at 9.7 assuming the size of the nc-Si is always a constant value of ~4.5 nm. The volume fraction of the nc-Si is also assumed to be a constant. When the SiO_2 thickness is 16 nm, it is observed that there is a difference of 2.13×10^{-4} F/m^2 between the capacitance of pure SiO_2 and the capacitance of SiO_2 embedded with nc-Si. As the SiO_2 thickness increases, the difference in the MOS capacitances reduces. This is mainly due to the increase of T_{oxide} but no changes in the capacitance of the nc-Si + SiO_2 layer. Even though the variation in MOS capacitance is small, this effect cannot be neglected. For example, when the SiO_2 thickness is 30 nm, there is still 5.7×10^{-5} F/m^2 difference between the SiO_2 and the SiO_2 with nc-Si. Such differences will become more significant when the nc-Si dosage increases.

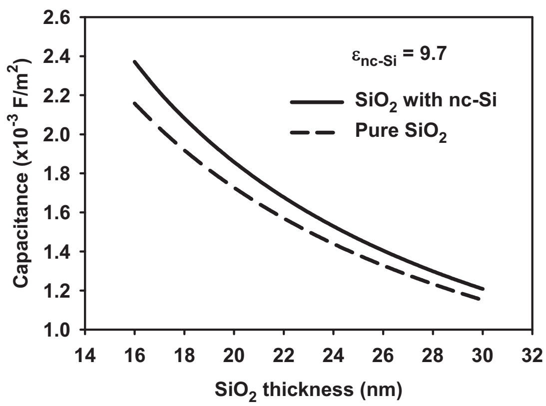


Figure 6: Total MOS capacitance of SiO_2 film with and without nc-Si as a function of different SiO_2 thickness. As the SiO_2 thickness increases, the capacitance difference between SiO_2 with and without nc-Si reduces.

4 CONCLUSION

The static dielectric constant of nc-Si embedded in SiO_2 matrix has been determined based on C-V measurements and Maxwell-Garnett EMA. For the nc-Si with a mean size of ~4.4 nm, the dielectric constant so determined is 9.6, being consistent with a theoretical prediction. This value is significantly lower than the static dielectric constant (11.9) of bulk crystalline Si. This result indicates the significance of nc-Si size effect. On the other hand, the influences of nc-Si distribution and the SiO_2 thickness on the MOS capacitance are also being presented. These results are important for future design and modeling of nc-Si-based memory devices

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