SUMMARY OF Ph.D. DISSERTATION

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Title

Enhanced diffusion of silicon and boron in thermal oxides formed on silicon substrates

Abstract

Thermal silicon oxide (SiO_2) is the most important gate insulating material in the silicon (Si) MOSFET technology today. The thermal Si oxide also plays an important role in the development of next generation gate insulator materials (e.g., high dielectric constant materials) because it continues to exist as an interfacial layer between the new gate material and Si wafer. The improvement of MOSFET performance has been achieved in the past by miniaturization. However, with the gate length reaching 100 nm and below, it is becoming increasingly difficult to realize thinner gate insulators and smaller channel lengths while maintaining the normal state of device operation. Lack of a precise atomic level picture of thermal oxidation mechanisms is interfering with development of future nanoscale thermal oxides. A phenomenon such as diffusion of boron (B) from the top polycrystalline silicon gate electrode to the Si channel region through SiO_2 gate insulator is smearing the well-defined channel in Si.

In order to overcome these problems, experimental investigations of Si and B diffusions in thermal SiO_2 formed on Si wafers followed by complete numerical modeling of the data were performed in the present study. The precise knowledge of Si self-diffusion in SiO_2 is indispensable for the development of future gate insulator architecture. Understanding of the B diffusion in SiO_2 is important to prevent the smearing of the channel region. In this study, ^{30}Si stable isotopes and B impurities embedded in isotopically enriched $^{28}SiO_2$ were employed as diffusion markers, and the diffusion of Si and B in SiO_2 as a function of the diffusion annealing temperature, annealing time, and thermal oxide thickness were investigated with and without surface silicon nitride (Si_3N_4) layers placed on the SiO_2 films. The depth profiles of ^{30}Si and B before and after annealing were determined by secondary ion mass spectrometry (SIMS). As a result, Si diffusivity obtained without surface nitride does not depend on the thickness of the SiO_2 film and agrees with the previously reported value of Si diffusivity in the bulk quartz. Such Si diffusivity remains the same for a variety of oxygen partial pressures in the annealing atmosphere, when there is no nitride layer on the top. On the other hand, when the nitride layer is placed, the Si diffusivity was found to increase as the thickness of the SiO_2 film is reduced. In order to understand this phenomenon quantitatively, we proposed a new picture in which SiO molecules generated at the SiO_2/Si interface due to $SiO_2+Si\rightarrow 2SiO$ reaction diffuse into the SiO_2 layer and enhance the Si diffusivity. Numerical simulation conducted based on this model for our variety of experimental conditions yield very good quantitative agreement with the experimental results, supporting the hypothesis used to developed the model. Similar experimental results were obtained for B diffusion in SiO_2 depending on the presence of the surface nitride layer, and the model assuming SiO enhancing the diffusion of B in SiO_2 reproduce our experimental results quantitatively.

In summary, we have performed experiments probing Si and B diffusion in SiO_2 formed thermally on Si wafers, and discovered that SiO molecules generated at the SiO_2/Si interface enhanced the Si and B diffusion when the nitride cap was placed. A unified mathematical model describing the correlated diffusion of Si and B developed in this study should be incorporated in the next generation Si process simulation software in order to increase the precision of the simulated outcome. It will be also of great interest in the future to develop new nanoscale Si fabrication technique utilizing the role of SiO defects.