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Modeling of the carrier mobility at the silicon oxynitride-silicon interface

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ABSTRACT

The main issue which is yet to be resolved in further developing the Surface Channel MOSFETs (SCMOSFETs) is understanding and eliminating detoriation of the carrier mobility at the insulator-semiconductor interface. The main factor causing this detoriation is hole and electron trapping-detrapping. One of the ways recently suggested of minimizing hole and electron trapping-detrapping at the Si-SiO_2 interface involves replacing the SiO_2 by silicon oxynitride (SiON). However degradation of MOSFETs, which have oxynitrides as gate dielectric, caused by trapping of hot electrons from the channel, is still found.

1. INTRODUCTION

The electrophysical parameters of the insulator-semiconductor interface are needed in order to determine the parameters of the transport carriers in the channel, and in paticular the main parameters for models of MIS devices – carrier mobility in the inversion layer. The latter has been the subject of intensive investigation since the 1960s.

Two fundamental problems in this field are (a) developing the technology for measuring the structures, and (b) interpreting the results of these measurements.

a) accuracy of modern methods for identifying mobility is largely dependent on accuracy in determining flat-band voltage U_{FB}. Accuracy in determining U_{FB} is, in turn, dependent on accuracy in determining such interface parameters as doping profile, the energy distribution of the traps and work function difference;
b) up to now it was believed that effective carrier mobility must be modeled by taking into account Coulomb, phonon and roughness scattering of the insulator- semiconductor interface with the help of the Mathiesen' rule, according to which these mechanisms are independent.

However measurements show that electron and hole mobility in the inversion layer are dependent on charge concentration both in the inversion layer and in the depletion region, but do not depend on their combination, which is not in keeping with the Mathiesen rule.

The main reasons for this divergence are that the influence of the interface structure on carrier transport is not taken into account, and over-simplifications occur.

Two examples of the latter are:

i) existing models of mobility are based in essence on a relaxation approximation of in the BTE;
ii) quantum effects in the inversion equation are not taken into account in these models.

Both these approximations cease to apply in the channel sizes currently obtainable and in the case of large dependent concentrations at the surface.

Therefore among the fundamental problems which need to be resolved in order to develop a model for transport mobility in the SCMIS transistor channel are the following:

i) the development of methods to solve BTE without any approximations;
ii) identification of a doping profile at the interface with a level of efficiency enabling their implementation.

Mechanisms for carrier transport, in particular, for scattering and for generation-recombination are clearly dependent on the structure of the insulator – semiconductor interface.

The structure of this interface is determined in the first instance by the mechanisms for the formation of the isolation layer. As a result of recently research into these mechanisms, significant progress towards the construction of a physical and chemical model has been achieved. Agreement of several parameters of this model with the parameters of an electrophysical model, which were determined using the modified conductance method was found. This confirms the dsirability of carrying out further work in integrating both approaches (the physical – chemical and the electro-physical) in order to model this interface.

In the oxydation procedure one key process is the transportation of atoms and particles.

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The oxynitrides have both advantages over SiO_2 (improved hot-electron immunity, higher charge to breakdown and suppressed boron diffusion) as well as shortcomings (degradation of MOSFETs with oxynitride as gate dielectric is still observed; considerably more interface states created for oxynitrides per injected hole than with SiO_2, more vulnerable to hole bombardment). Classical electric methods of investigations of mobility related phenomena are restricted because the relatively low mobility of the trapping carriers limits electroconductivity[1-13]. In order to assess the possible explanations both for these phenomena and for the nature of the defects, which have been proposed, a study of the electronic structure of a MOS system, using silicon oxynitrides as gate oxide, based on a first-principle molecular dynamic method, was carried out. A satisfactory explanation for the above-mentioned issues is crucial for constructing a model of carrier mobility.

We present a method which employs a band energy approach with molecular dynamic cluster optimization, the latter taking into account various structural modifications related to the non-stoichiometry of nanoclusters. We simulated the influence of chemical composition on the trapping properties of defects in siliucon oxynitride. Clusters with different numbers of oxygen and nitrogen atoms in the second coordination sphere were considered.

By calculating the differences between the total energy of clusters in different charge states, we determined the energy gain for hole or electron trapping in the case of different types of defects, and the dependency of this gain on composition and cluster size. Thermal delocalization of the energy level of traps was calculated. On the basis of these results, we propose models for the trapping (localization) and detrapping (delocalization) of electrons on different kinds of defects in SiO_xN_y and Si_3N_4. Mechanisms for creating different kind of defects, e.g. Linking two-fold coordinated nitrogen atoms with an unpaired electron, are proposed.

In order to determine the parameters of the oxynitride-Si system, non-linear optical methods, in particular photoinducing second harmonic generation (PISHG) were used.

2. ENERGY BAND STRUCTURE

The films were deposited by thermal low pressure chemical vapor deposition (LPCVD) on a silicon(111) substrate. The entire process was carried out using an ultra high vacuum chamber with pressure of about (4 x 10^{-8}) bar. The silicon(111) substrate is heated by radiation from a tungsten lamp. Such equipment enables acceleration of the evaporation process.

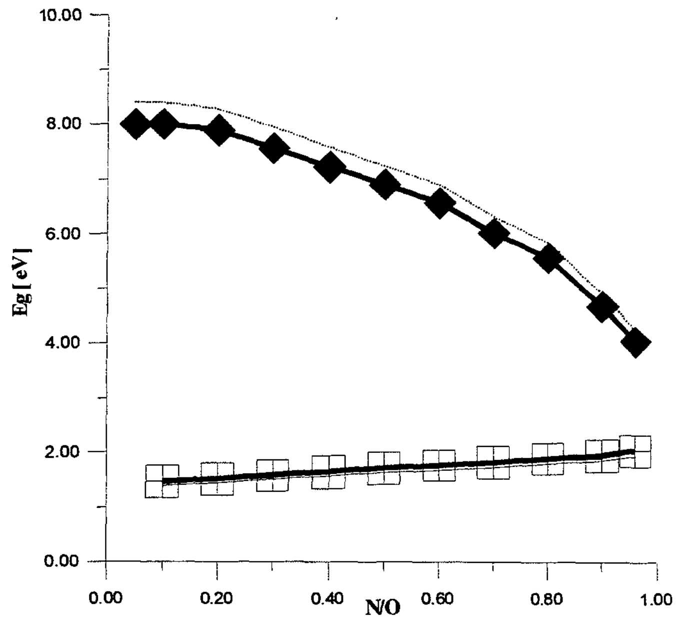

Fig. 1. Dependence of the energy gap E_g and refractive index n on the N/O ratio. ◆ - E_g measured; □ - n measured.

High-purity gases (chlorosilane - SiH2Cl2, ammonia - NH3, and nitrogen monoxide - N2O), the contents of which can be controlled with precision up to 0.2%, are used as a source for this process. The N/O ratio is changed by continuously varying the N2O/NH3 source/gas ratio. The growth rate, which is dependent on the N/O ratio, is selected in accordance with the Habraken rule. On the basis of the calculations carried out, the dependence of the band energy structure on the parameters of the oxynitride-silicon (SiON-Si) system was calculated. In Fig. 1 the calculated dependence of the energy gap E_g and refractive index n on the N/O ratio is presented, as well as the corresponding results of measurements[15]. One can see that the band energy gap decreases with a decreasing of nitrogen content. Good agreement between the calculated and experimentally evaluated parameters validates the adopted model of simulation.

In Figure 2 calculated dependence of the energy gap on the N/O ratio and film thickness is presented[16]. One can see that both the N/O ratio, as well as the film thickness, form modulated-like dependencies.

These dependencies reflect, as it were, a kind of "competition" between long-range bulk-like crystalline ordering, two-dimensional intersurface disorder and electron-phonon near-the-surface non-centrosymmetry. Analysis showed that the dependencies on film thickness of both the top of the valence band (VB), as well as of the bottom of the conduction band (CB), are non-periodic. The dependence on film thickness was found to be entirely different for the VB and the CB. This reflects the different influence of electron-phonon anharmonicity on the models considered, and the role of electron-phonon interactions on long-range ordering

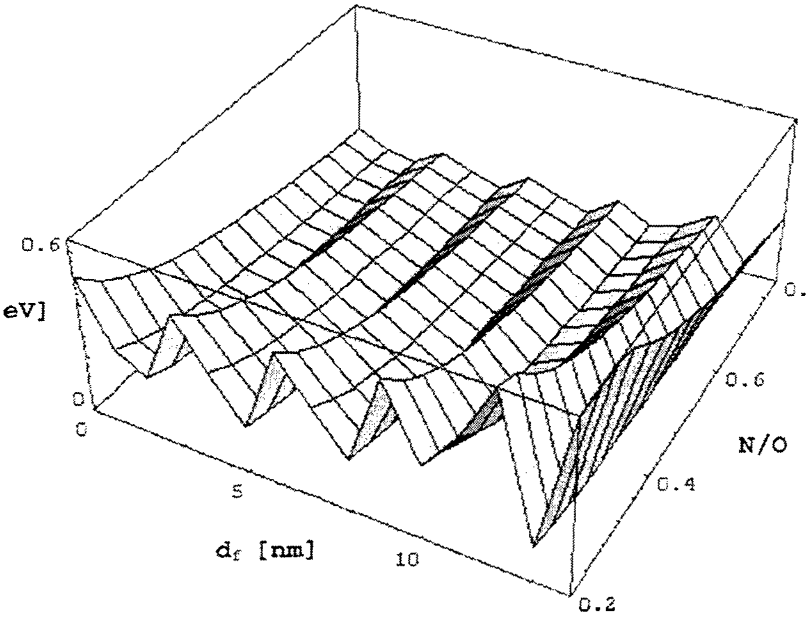

Fig. 2. Dependence of the band structure on N/O ratio and film thickness d_f.

3. GEOMETRY STRUCTURE

The results of molecular dynamic simulations of the O-Si and N-Si distances in relation to the N/O ratio and film thickness, carried out using the method described above are presented in Figure 3.[16] It can be seen that an increase in film thickness leads to an increase in the oxygen-silicon distance of between 0.16 and 0.28 nm. For an N/O ratio of approximately 0.015, the oxygen-silicon distance achieves its maximum at a thickness of about 28 nm. A further increase in the N/O ratio leads to a shift of the observed maximum positions towards the lower thickness (up to 16.5 nm for an N/O of about 1.0). The existence of maxima would also seem to reflect a kind of 'competition' between long-range ordering of the silicon crystalline surface, and random amorphous-like disordering due to the substitution of the nitrogen and oxygen in the silicon positions. Oxygen and nitrogen cause opposite changes in the charge density distribution, and, therefore, in the interface electrostatic potential distribution near the oxynitride-silicon<111> (SiON-Si < 111>) interface. The dependence on film thickness for the nitrogen-silicon (N-Si) distances is significantly different from that for oxygen-silicon (O-Si) distances. In the first place, one can see in Figure 8 two thickness maxima. The first has a value of about 0.21 nm for a film thickness range of 10-16 nm, the second of about 0.28 nm within the thickness range 18 nm-24 nm. The appearance of the two maxima suggests the existence of two possible minima of the local cluster total energy for the nitrogen-silicon (N-Si) distances, in contrast to the oxygen-silicon (O-Si) distances.

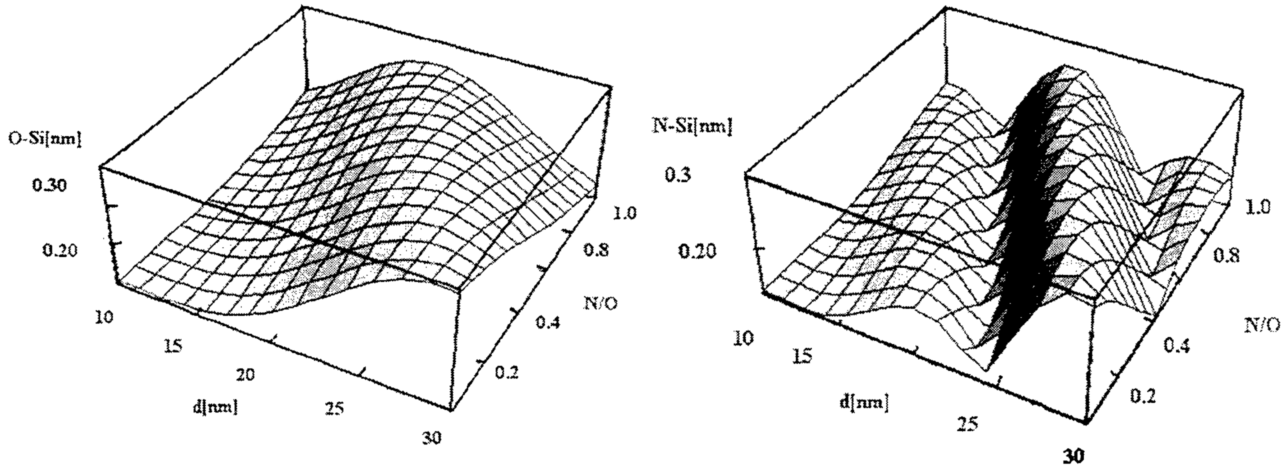

Fig. 3. Molecular dynamics geometry optimization of the O-Si and N-Si distances versus the film thickness d and the N/O ratio.

4. CONCLUSIONS

Nitridation leads to an increase in concentration of interface states and 1/f noise. This is seen particularly in the case of nitridation in NH_3 where trapping centers are introduced through the hydrogen, and with oxides formed in an N_2O atmosphere, due to deterioration in the structure of the interface layer as a result of an initial increase in the speed of formation. A significant decrease in carrier mobility for lower strengths of the electric field has also been found in MOS transistors with an n channel as a result of nitrogen implantation before oxydation. On the other hand, no increase in carrier mobility was observed for higher electric fields. However where formation occurred in an N_2O atmosphere, there was no significant decrease in mobility for lower strengths of the fields, while there was a detectable increase in mobility for higher fields. In the case of SiON layers formed through a PECVD (plasma .enhanced chemical vapor deposition) procedure, a significant decrease in mobility for lower strengths and a detectable increase for higher strengths have been established, together with lower hot-hole immunity, in comparison with SiO_2 of the interface SiON-Si layer.

In the carrying out the present work I found a number of discrepancies in the explanation for the above-mentioned specific observations regarding the influence of nitrogen on the properties of the SiON-Si system. These discrepancies make it practically impossible to give a uniform description of carrier transport in transistor channels with SiON gate isolation. A model of the influence of nitrogen on the properties of M-SiON-Si structures, based on an investigation both of the energy structure, as well as of the geometry structure, of the SiON-Si interface region is needed. In order to determine the influence of nitrogen on the proprties of the SiON layers and on the properties of the interface SiON-Si layers, the ratio of the nitrogen concentration to that of oxygen (N/O) must be established, together with influence of nitrogen atoms on the geometry structure (for example, the distances N-Si and O-Si) and the energy structure of both the SiON, as well as the interface SiON-Si layer.

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