

Oxidation Simulation and Growth Kinetics of Thin SiO_2 in Pure N_2O

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Abstract

This paper reports the oxide growth behavior of silicon in an N_2O ambient using conventional furnace method. With all three different wafer orientations and wider temperature and time ranges used in our experiments, it has been found that the oxide growth can be simulated by the linear-parabolic model. This is in direct contrast with previous reports that the oxide growth is self-limited, or it was described only by the linear rate constant in oxidation.

1. Introduction

NH_3 -Nitrided SiO_2 has been studied in the past ten years to improve the electrical properties of silicon dioxide layer. A re-oxidation is required immediately after nitridation step to minimize the high electron trapping efficiency and high electron trap generation rate due to a large amount of hydrogen atoms (H) in the oxide. Though reoxidation has been proved to be effective in reducing hydrogen concentration, the optimization of this process is complicated. Recently there has been tremendous interest in N_2O oxidation using either conventional furnace [1] or rapid thermal processor [2] to form high quality gate dielectrics. The growth of SiO_2 was reported to be self-limiting [3]. However, we have found the non-saturation growth behavior over a wide range of temperatures and different crystal orientations in N_2O oxidation [4].

In this work we present an oxidation model and discuss some simulation results.

2. Experimental

N_2O oxidation was performed in a conventional resistive-heated furnace in high purity gas (moisture less than 0.5 ppm) (>99.9995%) for (100), (111) and (110) oriented Si substrates. Oxide thicknesses were measured using ellipsometer with an assumed refractive index of 1.462. They were also confirmed by a high-frequency C-V measurement with less than 5% discrepancy. Fig. 1 shows oxide thickness versus oxidation time for (111) Si over the temperature from 900 C to 1100 C. (100) and (110) oriented substrates exhibit similar behavior but with different thicknesses.

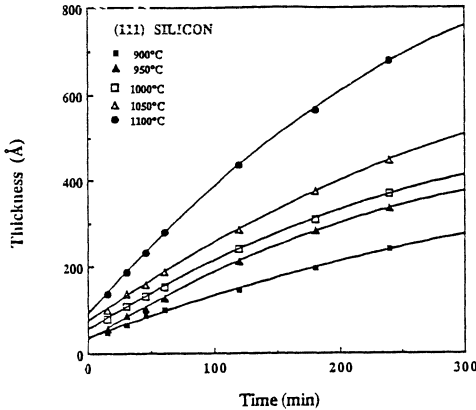


Fig. 1 Oxide thickness vs. oxidation time for (111)-oriented silicon

3. Results and Discussion

Several important features can be observed from experimental results. First, the growth of SiO_2 was found to be not self-limited. Second, the N_2O oxidation rates are much slower than those in dry O_2 . Third, the (110) and (111) oxidation exhibits the "crossover" behavior in which the (110)-oriented silicon has a higher oxide growth rate than (111)-oriented wafer in the initial oxide growth. After oxide thickness exceeds 175 Å, the (111)-oriented silicon has highest growth rate. This phenomenon was previously also observed in the dry oxygen oxidation [5].

Since oxygen from N_2O decomposition at high temperatures ($N_2O \rightarrow N_2 + 1/2O_2$) is primarily responsible for the oxidation and NO is responsible for nitrogen incorporation in the Si/SiO₂ interface [6] which may retard the oxide growth, the rather complex oxide growth behavior in N_2O can be modeled by using oxidation of silicon in diluted dry oxygen. Empirically it was found that the growth rate in pure N_2O is essentially identical to that in 10% dry O_2 in argon over the temperature range from 900 C to 1000 C. The experimental data of 10% O_2 /Ar [5] are compared with N_2O data as shown in Fig. 2.

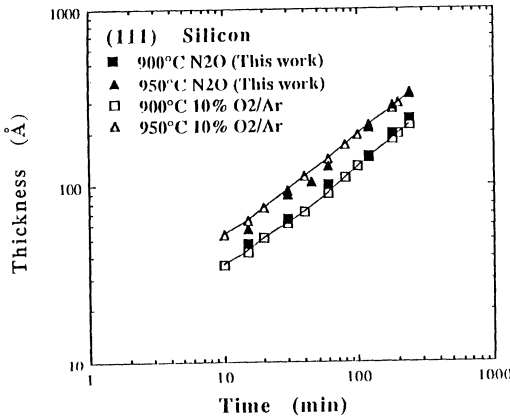


Fig. 2 Comparison of N_2O oxidation and 10% dry O_2 -argon mixture oxidation for (111)-oriented silicon

Both N_2O and 10% O_2 in argon follow the same linear-parabolic model. Based on the experimental data, except for the very short oxidation time, the linear rate constant (B/A) and parabolic rate constant (B) can be determined and are plotted as a function of temperature as shown in Fig. 3 and Fig. 4 respectively.

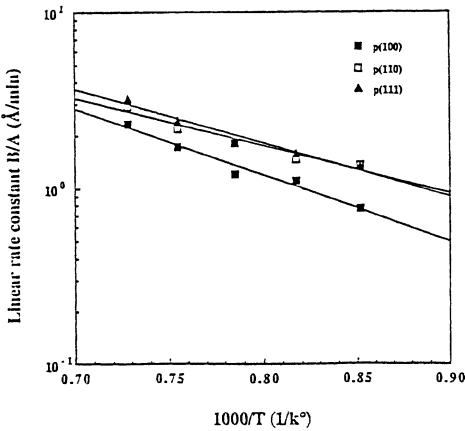


Fig. 3 Linear rate constant B/A as a function of temperature for (111), (100), and (110)-oriented silicon

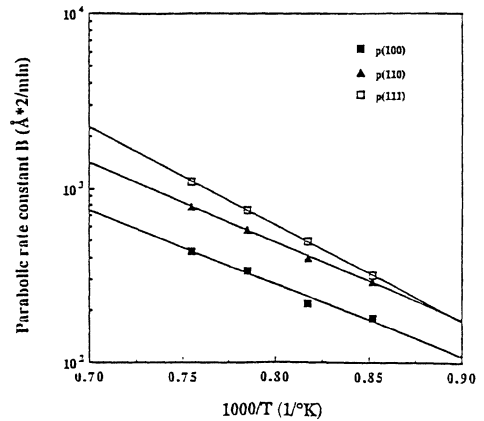


Fig. 4 Parabolic rate constant B as a function of temperature for three different orientations

Previous study of N_2O oxidation covers only a limited temperature range, time and oxide thickness [7]. Therefore the growth behavior in that case was characterized only by the linear rate constant (B/A). However it is evident that as oxidation time gets longer or oxidation temperature is greater than 1000 C, the single linear rate constant representation is inadequate. In order to fit a much broader temperature range and oxidation time, parabolic growth behavior must be considered. The activation energy E_a of B/A and B for all three orientations is shown in Table 1.

Table 1. Activation energy E_a of B/A and B for N_2O oxidation in the Linear-Parabolic Model

	(100)	(110)	(111)
B/A	1.005	0.734	0.860
B	0.800	0.880	1.100

4. Summary

Using the experimental data, we have shown that the oxide growth of silicon in N_2O oxidation is not self-limited and an empirical model has been proposed to cover both linear and parabolic regions of oxide growth over a wide temperature and time

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