Effect of Strain on the Oxidation Rate of Silicon Germanium Alloys

Mohamed A. Rabie*, Steven Gou**, Yaser M. Haddara***, Andrew P. Knights****, Jacek Wojcik*****, and Peter Mascher******

*Electrical and Computer Engineering, McMaster University, Hamilton, ON, Canada, rabiema@mcmaster.ca

Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, sgou@phas.ubc.ca

***Electrical and Computer Engineering, McMaster University, Hamilton, ON, Canada, yaser@mcmaster.ca

****Engineering Physics, McMaster University, Hamilton, ON, Canada, aknight@mcmaster.ca

*****Engineering Physics, McMaster University, Hamilton, ON, Canada, wojcikj@mcmaster.ca

******Engineering Physics, McMaster University, Hamilton, ON, Canada, mascher@mcmaster.ca

ABSTRACT

We report on a series of experiments in which a strained $Si_{0.95}Ge_{0.05}$ layer 600Å thick was oxidized along with relaxed SiGe layers and Si samples. In this work, we observed that the oxidation rate of the strained SiGe layer is always much higher than the relaxed model expectations. We also observed that the rate is higher than that of relaxed SiGe layers with higher Ge concentration oxidized at similar temperatures. We attributed this increase in the rate of oxidation to the effect of strain in the SiGe layer. To confirm our hypothesis, we oxidized strained SiGe layers together with relaxed SiGe layers of higher concentration. We observed that the strained SiGe layer compared with relaxed sample has a thicker oxide despite the lower Ge concentration. We conclude that the strain in the SiGe layer causes a further increase in the oxidation rate.

Keywords: SiGe, oxidation, modeling, strain.

1 INTRODUCTION

Thermal oxidation of SiGe is a necessary process step for many applications in which SiGe is used. The oxidation process of SiGe results in a low quality oxide due to an undersirable Ge-rich layer below the oxide as well as high fixed charge density and trap density at the oxide/substrate interface [1 and references therein]. To improve the quality of the oxide, the physics of the oxidation process has to be well understood. One factor that has not been thoroughly considered before is the effect of the strain on the oxidation process. To understand the effect of strain on the oxidation process we conducted a number of oxidation experiments on strained SiGe samples as well as relaxed samples.

It is well established in the literature (see [1-2] and references therein) that the oxidation rate of SiGe increases with the increase in temperature and the increase in the concentration of Ge. Our previously published model [1] was able to quantify this increase to a high degree of accuracy. The experiments we carried showed that the strained SiGe layers oxidize at a higher rate than relaxed SiGe layers at similar temperatures and Ge concentration. The experimental results were also compared to the relaxed oxidation model expectations [1]. We were able to reach a conclusion that strain enhances the oxidation rate of SiGe. The faster oxidation rate can be attributed to a weaker Si-Ge bond in the case of strained SiGe. This new conclusion can help us to understand the mechanism involved in enhancing the oxidation rate of SiGe over that of Si. Three mechanisms have been previously proposed [1]. One of them is the weaker Si-Ge bond compared to Si-Si bond. Our conclusion confirms that the weaker Si-Ge bond is one of the causes of the enhancement in the oxidation rate of SiGe compared to that of pure Si. Understanding the effect of the bonding factor on the reaction rate will help in achieving more accurate physical and mathematical modeling for the SiGe oxidation.

In the following section we describe the experiments that were conducted as well as the experimental challenges we faced in achieving accurate results. The experimental results are shown and discussed in the last section of this paper.

2 EXPERIMENTAL PROCEDURES

Initially, a strained $Si_{0.95}Ge_{0.05}$ was oxidized at 820°C in a tube furnace. The SiGe layer was 600Å thick on top of a Si substrate. The wet oxygen mixture was prepared by bubbling oxygen through boiling deionized water at 1 SCFH flow rate [3].

When the enhancement in oxidation rate of strained SiGe was observed a number of experiments were conducted to make sure that the effect of furnace calibration on the oxidation rate is minimal. That set of experiments resulted in a number of precautions that were taken with the later experiments. The temperature of the DI water was adjusted just below the boiling temperature to ensure that the wet mixture will result in wet oxygen rather than a mixture close to dry O_2. We ensured that the furnace is dry before every oxidation experiments. Water droplets from the furnace resulted in islands in the oxide. The samples orientation in the furnace was always the same to have the same exposure for all the oxidized samples.

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After this set of calibration experiments, more oxidation experiments were conducted. In the new set of oxidation experiments Si was always oxidized with SiGe. Since the oxidation rates of pure Si are well established in the literature. Si served as an indicator for the actual furnace temperature. The initial experiment was repeated and the results came close to the first run. A number of other experiments were conducted for various temperatures and for different periods of time. For the experiment done at 780˚C, a relaxed CZ grown $Si_{0.905}Ge_{0.095}$ was oxidized with the strained $Si_{0.95}Ge_{0.05}$ to recognize the effect of strain with no doubt.

3 RESULTS AND DISCUSSION

Figure 1 shows the experimental measurements for the oxide thickness of the strained $Si_{0.95}Ge_{0.05}$ compared to the predictions of the relaxed oxidation model [1] at 820˚C. It is clear that the rate of oxidation is much higher than the expectations by the model. The results were then compared to the oxidation rate of $Si_{0.86}Ge_{0.14}$ reported in the literature [2] at a close temperature: 800˚C. The relaxed model predicts the results reported in the literature to a high degree of accuracy (not shown in the figure). Yet, our experiments show a higher oxidation rate than that predicted by the model. Furthermore, our experimental results show a higher oxidation rate than that reported by LeGoues et al. [2] despite a higher Ge fraction in LeGoues et al.'s experiment (14% compared to 5%). It is well known that the oxidation rate of SiGe increases considerably with the increase in the Ge content [1 and references therein]. It is also well known that the rate increases with the increase in temperature [1 and references therein]. Our previously reported model [1] was able to quantify these effects to a high degree of accuracy. Despite these facts, the oxidation rate for the 5% SiGe at 820˚C was higher than that for the 14% SiGe. This contradicts with the model expectations. The higher oxidation rate was attributed to the effect of strain on the oxidation rate.

To justify this conclusion; further experiments were conducted. The results of those experiments are shown in table 1. It is clear from the table that the experimental results for the oxide thickness on the strained $Si_{0.95}Ge_{0.05}$ are much higher than the expectations of the relaxed model. In the table the experimental measurement for the oxide thickness of the relaxed $Si_{0.905}Ge_{0.095}$ is also shown. This sample has been oxidized simultaneously under the same furnace conditions with the strained $Si_{0.95}Ge_{0.05}$. Despite a higher Ge fraction, the oxide thickness was larger for the relaxed sample. This is evidence that the strain enhances the oxidation of SiGe alloys.

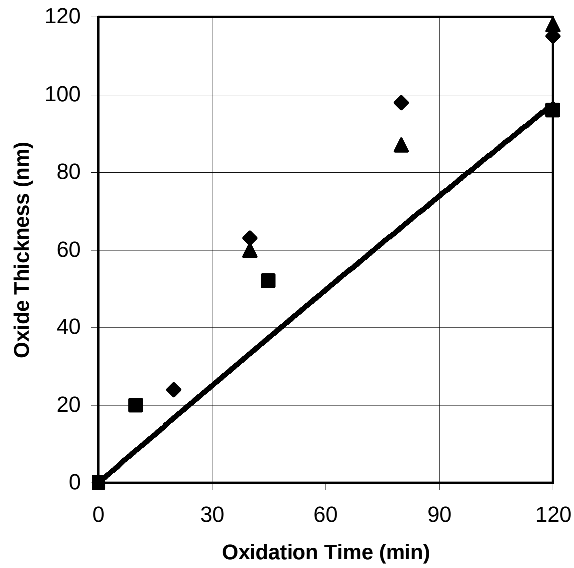

Figure 1: Oxidation rate of strained $Si_{0.95}Ge_{0.05}$ layer 600Å thick at 820ºC (♦: RBS; ▲: ellipsometry) compared to oxidation rate of a relaxed $Si_{0.86}Ge_{0.14}$ layer at 800ºC (■: ellipsometry) [2]. The experimental data is also compared to the relaxed oxidation model [1] expectations for 5% Ge at 820ºC (line).

Three mechanisms were proposed previously to explain the enhancement in the oxidation of SiGe alloys over pure Si [1]. The first mechanism is the change of the path of the oxidation reaction. GeO is formed first and then Ge is replaced by Si forming SiO_2. That path of the reaction is faster than the direct oxidation of Si. The second mechanism is the suppression of the injection of interstitials. Interstitials are injected during the oxidation process of pure Si which results in slowing down the oxidation process. The Ge atom is larger in size than the Si atom. It was experimentally shown that the injection of interstitials is suppressed during the oxidation of SiGe [4]. This will enhance the oxidation rate if the injection of interstitials was a rate limiting step in the case of oxidation of pure Si [1].

The third mechanism which contributes to the enhancement in the oxidation rate of SiGe alloys is the weaker Si-Ge bond compared to Si-Si bond. This means that the Si-Ge bond breaks easier than the Si-Si causing an enhancement in the oxidation rate. Our results support this hypothesis. Strained bonds are weaker than relaxed bonds. We observed an enhancement in the oxidation rate of strained SiGe over relaxed SiGe. This can be attributed to the weaker Si-Ge bond in case of strained SiGe. Similarly, we can conclude that the oxidation of relaxed SiGe is enhanced over pure Si due to the weaker Si-Ge compared to the Si-Si bond.

Temperature (ºC)	Time (min)	Experimental Thickness (Å)	Relaxed Model Expectations A (Å)	Closest Relaxed Experimental Measurements (Å)	Relaxed Model Expectations B (Å)
715	30	50	40	–	–
780	50	550	222	342[a]	322
805	40	464	253	520[b]	550
845	120	2262	1435	–	–

Table 1: Results of oxidation of strained $Si_{0.95}Ge_{0.05}$ layer 600Å thick at different times and temperatures compared to the relaxed oxidation model [1] expectations (A) at the corresponding times and temperatures. The results are also compared to the closest relaxed experimental measurements available. The model expectations (B) for those experimental results are also reported.

[a] This result comes from our own experimental measurements for a relaxed CZ grown $Si_{0.905}Ge_{0.095}$ oxidized for the same time and at the same temperature with the strained $Si_{0.95}Ge_{0.05}$ layer indicated in that row.

[b] Oxide thickness for the relaxed $Si_{0.86}Ge_{0.14}$ oxidized for 45 minutes at 800 ºC as reported by [2].

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