Paper

Oxidation kinetics of silicon strained by silicon germanium

Jarosław Grabowski and Romuald B. Beck

Abstract—This paper reports on the studies of oxidation kinetics of silicon strained by silicon germanium layers. Experimental results of natural, chemical and thermal oxide formation are presented. The oxidation rates of silicon strained by SiGe layers have been compared with the rates of pure Si oxidation. The oxidation kinetics was studied using the parallel model proposed by Beck and Majkusiak. This model was fitted with good result to the obtained experimental data and the parameter that is most probably responsible for the strain effect was identified, as well as its dependence on Ge content in the SiGe layer.

Keywords—oxidation, kinetics, modeling, silicon, silicon germanium.

1. Introduction

Constant increase of speed in every IC generation is an obvious trend in the development of microelectronics. So far it has been achieved mostly by continuous down-scaling of devices over the years. Using silicon germanium is another way to reach this goal (e.g., [1, 2]). A thin, relaxed layer of SiGe alloy can induce enough strain in a silicon cap to improve carrier mobility (e.g., [3]). However, introduction of any new material into IC production requires that both, processing and its successful integration, have to be ensured.

This paper covers selected types of strained Si oxidation, namely natural, chemical and thermal oxidation.

2. Experimental and results

In our experiments, samples containing silicon substrate covered with relaxed SiGe buffer (with varied Ge content) and topped with Si cap were used. The samples were fabricated at the University of Warwick by means of either molecular beam epitaxy (MBE) or low pressure chemical vapor deposition (LPCVD). We used J. A. Woolam spectroscopic ellipsometer to investigate the thickness of every oxide.

In the first part of the study the thickness of natural oxide grown spontaneously on the silicon cap strained by the underlying SiGe buffer was measured using spectroscopic ellipsometry. In chemical-oxidation experiments (second stage) we used SC1 mixture (H_2O-NH_4OH-H_2O_2 5:1:1). Samples were kept in this mixture for 10 min at 90°C. The obtained results (natural oxide and chemical experiment) are presented in Table 1.

Table 1
Results of natural and chemical oxide thickness measurements

Fabrication method	SiGe thickness [nm]	Ge fraction [%]	Native oxide thickness [nm]	Chemical oxide thickness [nm]
Si ref.	–	–	1.7	2.0
LPCVD	7	5	1.5	2.0
LPCVD	7	10	1.5	1.9
LPCVD	7	20	1.5	1.9
LPCVD	7	30	1.6	1.9
MBE	18	14	2.0	8.4
MBE	19	13	4.2	–

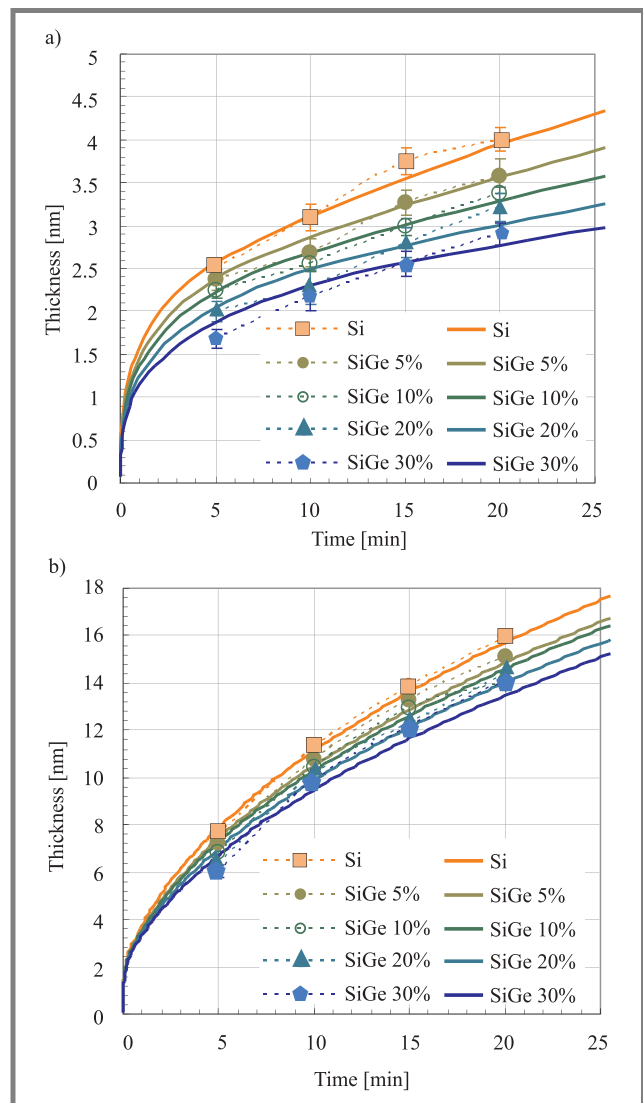

Fig. 1. Dependence of the kinetics of thermal oxidation at: (a) 800°C and (b) 900°C on Ge fraction in the SiGe layer (dots – experiment, lines – model).

In the third stage of this study, thermal oxidation experiments were performed at two different temperatures (800°C and 900°C) in dry oxygen with 0.25 l/min oxygen flow. Figure 1 shows the thickness (measured by means of ellipsometry) of thermal oxides grown at 800°C and 900°C, respectively.

The parallel model proposed by Beck and Majkusiak (B-M) and presented schematically in Fig. 2 has already been used

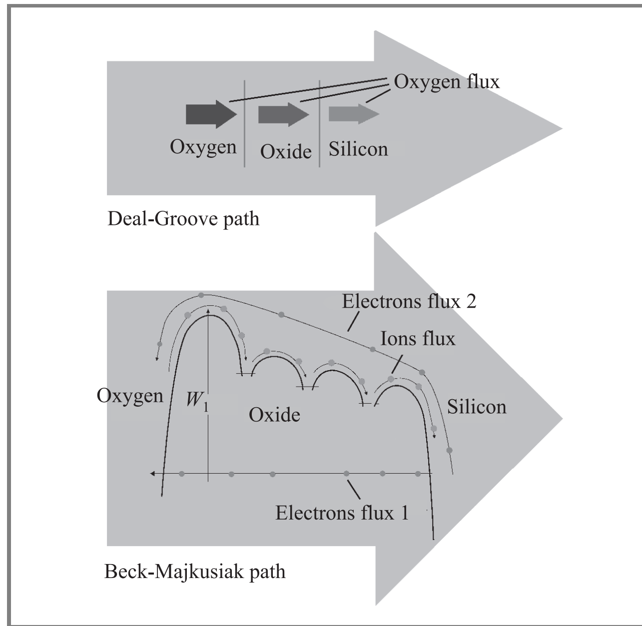

Fig. 2. Oxidation kinetics model proposed by Beck and Majkusiak.

to model thermal oxidation kinetics (e.g., [4–7]). According to this model oxidation species are supplied to the reaction site by two parallel paths. The first one is described by the traditional 3-parameter Deal-Groove model [8]. The other, parallel path is the flow of oxygen ions. This flux is controlled by electrochemical effects (balance of oxygen ions flow to the reaction sites and electrons supply to the surface) and is described by seven additional parameters. The B-M model was fitted to all the experimental data obtained in this study (Fig. 1) and all of its parameters were determined. It appears that only one of these model parameters is critical for good fitting of the B-M model to the data obtained from samples with different Ge concentration in SiGe buffer. This parameter is the initial potential barrier height (W_1) for the flux of ions entering the oxide (see Fig. 2).

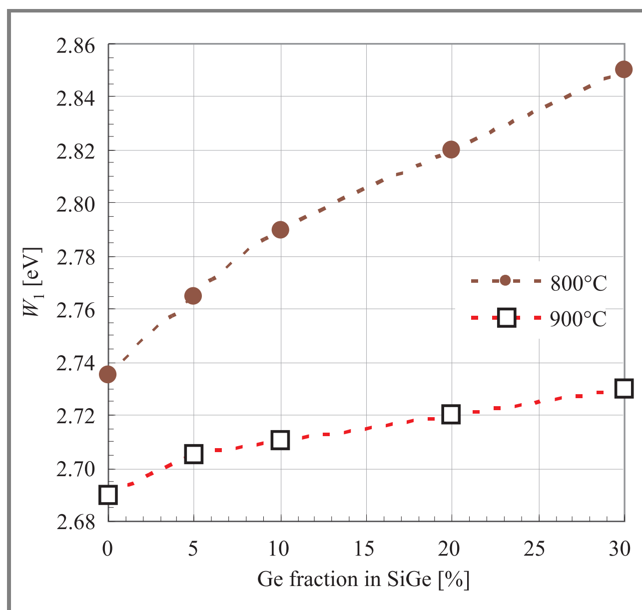

Fig. 3. Values of W_1 providing good fitting of the B-M model to the experimental data obtained from samples with different Ge fraction in the SiGe layer.

Figure 3 shows the values of the initial potential barrier height (W_1) that provide a good fit of the B-M model to the experimental data as a function of Ge concentration in the SiGe buffer for both studied temperatures. When Ge concentration and strain level in the silicon cap increase, the height of the initial potential barrier W_1 increases consistently for both temperatures.

3. Discussion

Significant differences in the natural and chemical oxide thickness are visible between MBE and LPCVD samples. This indicates that the method used for SiGe formation might have critical influence on its chemical and physical properties. Natural and chemical oxide thickness of LPCVD samples is almost independent of Ge concentration in the SIGe buffer. Very weak decrease of oxide thickness is observed with increasing Ge concentration. Relatively high oxide thickness of MBE samples might result from the strain induced in the silicon caps leading to higher oxidation rates.

In the case of LPCVD samples the results obtained in the course of thermal oxidation were similar to natural and chemical experiments. They show that strained silicon layers oxidize even more slowly than the reference Si wafers. It can be seen that when the strain increases (through the increase in Ge concentration in the SiGe layer), oxidation rate becomes lower.

In the B-M model, the initial potential barrier height (W_1) is the parameter responsible for the description of oxygen ions entering into the growing oxide. Therefore, a change of its value may mean a change of the growing oxide surface conditions (e.g., surface contamination). While the reasons for this effect are not clear, at least two hypotheses may be proposed.

First, germanium atoms may migrate from silicon germanium into the strained silicon cap and contaminate it. After oxidation these atoms may contaminate the newly formed oxide layer. The contamination of silicon to be oxidized also changes the conditions of the oxidation process (chemical reaction rate). The resulting changes in the oxidation rate may compete with the results of strain in the cap. Moreover, germanium outdiffusion from the SiGe layer

(due to high temperature during oxidation) tends to relax the strain in the cap. In such conditions the expected dependence of the oxidation rate on germanium concentration in SiGe should become weaker with increasing oxidation time. In fact this hypothesis seems to be confirmed by recent studies carried at the University of Warwick.

Second, it is possible that the B-M model is not suitable for strained samples. This would mean that good fitting of the B-M model to the oxidation kinetics affected by changes in Ge concentration in SiGe layer is merely a coincidence and that a parameter (or parameters) other than W_1 is really responsible for this effect. It should be mentioned, however, that the values of W_1 are in all cases physically meaningful and reasonable for the energy diagram assumed in the model, which would suggest that this hypothesis is less probable than the previous one.

4. Conclusions and summary

The presented results demonstrate that MBE samples exhibit higher oxidation rate than LPCVD ones in the case of natural and chemical oxidation experiments.

Oxidation rate of LPCVD samples is lower than that of reference Si wafers. It seems also that natural and chemical oxide thickness of LPCVD samples does not depend on Ge concentration in SiGe.

Thermal oxidation experiments (in the initial oxidation phase) show that increasing Ge concentration in the SiGe layer leads to lower oxidation rates for LPCVD samples.

The B-M model was used to study thermal oxidation kinetics. In this model only one parameter responsible for the observed changes in the oxidation kinetics was found. Although two different hypotheses explaining the correlation between this parameter and the observed strain effects were proposed, the recent study carried out at the University of Warwick seem to support only the first one.

Acknowledgments

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Romulad B. Beck – for biography, see this issue, p. 7.