VERSATILE N-TYPE PROFILE ENGINEERING BY CONTROLLING ARSENIC SURFACE SEGREGATION IN SILICON RPCVD

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ABSTRACT

With the purpose of controlling the incorporation of arsenic during RPCVD Si epitaxy, the surface segregation of As during low-temperature epi growth was investigated. Parameters such as the Si growth rate, As deposition rate and As incorporation rate, which in previous models were either not evaluated or assumed to be constant, were found here to depend on both the As surface coverage and the arsine partial pressure. Knowledge of these dependencies was employed in simultaneous As deposition and Si epi growth to obtain highly-controllable doping profiles by appropriate variation of the arsine partial pressure.

INTRODUCTION

Precise engineering of doping profiles can greatly improve the performance of Sibased devices, especially for microwave and RF applications. For example, in bipolar technology tailoring the collector with a non-uniform doping profile can enhance highfrequency behavior by, for example, improving the trade-off between linearity and ruggedness [1], or by increasing the maximum cutoff frequency f_T [2]. Moreover, for varactor diode-based circuit topologies, which have recently been presented as high-Q "distortion-free" tunable capacitive elements for RF adaptivity [3], there is an increasing demand for a wider tuning range. This requirement can be satisfied by the implementation of application-specific doping profiles that make it possible to achieve the desired capacitance-voltage characteristics. In particular, it is of great interest to fabricate hyper-abrupt junctions since they can provide a much higher voltage sensitivity than simple uniformly-doped layers, examples of which are given in [4] and [5].

For achieving this high degree of versatility and accuracy in fabricating profiles, insitu doping during CVD epitaxy is a technique that offers unmatched control. A procedure enabling fabrication of highly-doped and abrupt arsenic profiles in the silicon epilayer during Low-Temperature CVD was presented in [6]. Although the As surface segregation complicates the controllability of the doping concentration in the epilayer, this n-type dopant is very attractive since it combines low diffusivity with a high solubility in silicon, providing compatibility with existing processes and more freedom in doping range. Therefore, in view of these promising properties exact knowledge of the growth parameters is crucial.

In this paper we extend the model of [6] to the point of general applicability by employing simultaneous growth of low temperature epitaxial Si layers and As deposition. We present an improved description of As segregation during epi growth process, deriving from experimental data the dependences of parameters involved in the process on processing conditions.

CONTROLLING DOPING PROFILES BY UTILIZING DOPANT SEGREGATION

Previous studies have shown that As-doping during epi growth is dominated by the effects of As surface segregation [6], [7]. The segregation is not complete and a certain fraction of As atoms from the surface is during growth being incorporated into the epi layer. This results in a doping $N_d(x)$ proportional to the As surface coverage θ so that

$$N_d(x) = i_R N_{Si} \theta , \qquad (1)$$

where θ is expressed as a fraction of a full monolayer, $N_{Si} = 5 \cdot 10^{22} \text{ cm}^{-3}$ is the concentration of Si atoms in the lattice and i_R is the constant of proportionality called the incorporation rate.

Processes of epi growth and As deposition can be simply characterized by

$$dx = g_R dt \tag{2}$$

and

$$d\theta = d_R P_{As} dt , \qquad (3)$$

where x denotes epi thickness, g_R and d_R are growth and deposition rates, respectively, and P_{As} is the gas partial pressure of arsine (AsH₃) in the deposition chamber. To this set of equations, we add the continuity equation for the surface coverage

$$d\left(N_{ML}\theta\right) = -N_d\left(x\right)dx + N_{ML}d_R\left(\theta\right)P_{As}\left(t\right)dt,$$
(4)

where $N_{ML} = 6.8 \cdot 10^{14} \text{ cm}^{-2}$ is a surface density corresponding to a full monolayer on (100) surface, and dx and dt are related by (2). Left-hand side of equation (4) represents the change in the surface density of As atoms, the first term on the right-hand side represents As incorporation, and the second term stands for As deposition.

Our aim was to gain control over the process of simultaneous epi growth and As deposition in order to precisely shape the doping profile. To this aim, we have investigated functional dependencies of the incorporation, growth and deposition rates on the As surface coverage and arsine partial pressure, and in that way extended the above model. With that knowledge, we could numerically solve the set of equations (1)-(4) in order to obtain the $P_{As}(t)$ dependence that yields the desired $N_d(x)$.

EXPERIMENTS AND PROCESS DESCRIPTION

Samples were fabricated in the ASM Epsilon One epi reactor at reduced pressure of 60 Torr at 800°C with dichlorsilane and arsine as sources and with H_2 carrier gas flow of 50 standard liters per minute (slm). Wafers were baked before growth for 2 min at 1150°C for cleaning purposes. When removal of excess As from the surface was desired wafers were baked for 10 min at 875°C, followed by a growth of 5 nm of undoped Si and with repeated bake off step. Some of the samples were capped with a layer of undoped Si.

Samples were characterized by weighing the deposited Si and by C-V measurements to profile the as-grown As-doped layer. For the latter an Al/Si Schottky diode to the n-type Si was fabricated. In order to alleviate the limitations posed by reverse breakdown of the Schottky diode, the distance to the high-doped region of the As-doped profile was varied by plasma-etching to remove different Si top-layer thicknesses on different dies on the same wafer. In this way a larger part of the doping profile could be determined.

Three sets of experiments were designed. In the first set a sub-monolayer of As was deposited followed by epi growth without any arsine flow. This resulted in exponentially decreasing profiles, an example of which is shown in Fig. 1. The profiles have characteristic lengths inversely proportional to the incorporation rate. With the extracted incorporation rates the corresponding surface coverage values were calculated to obtain values for averaged deposition rates. This measurement technique was, however, not accurate enough to allow an accurate prediction of the dopant incorporation.

The second set of experiments employed growth with constant partial pressure of arsine (Fig. 2), and thus only investigates the dependency on coverage. Wafers were fabricated with different growth times, which enabled us to measure C-V profiles of different sections of the complete profile that is achieved with the longest growth time. In addition, weighing of each wafer yielded growth rate as a function of coverage and the shape of the doping profile yielded deposition rate as a function of coverage.

The third set of experiments employed growth with increasing partial pressures of arsine (Fig. 3). This provided us with the incorporation rate dependence on the arsine pressure, further explained in the following section. All three parameters were fine-tuned to achieve a good fit between the predicted profiles and the measured C-V profiles as seen in Figs. 2 and 3.

RESULTS AND DISCUSSION

Parameter dependencies

The following functional dependencies of parameters were extracted from the measurements. Our experiments were performed within the following ranges: $P_{As} \in (10^{-7}, 1.5 \cdot 10^{-5})$ Torr, $\theta \in (0.01, 0.16)$, and $N_d \in (3 \cdot 10^{16}, 2 \cdot 10^{18})$ cm⁻³. Due to the complicated fitting process, confidence intervals could not be evaluated.

The Si growth rate was found to be moderately inhibited by the As surface coverage,

$$g_R = \left(43 - 120\theta\right) \frac{\mathrm{nm}}{\mathrm{min}}.$$
 (5)

This growth rate corresponds to a H_2 carrier gas flow of 50 slm and dichlorsilane gas flow of 296 standard cubic centimeters per minut (sccm). The growth rate is determined by the impinging rate of DCS molecules with enough energy to be decomposed and the probability for the Si atom to remain at the surface (the sticking coefficient) [8]. The former is dependent on the partial pressure of DCS and on the temperature according to Boltzmann statistics. The latter can and generally will be different for a Si atom impinging on either a clean or an As covered Si surface. Therefore the average sticking coefficient and consequently the average growth rate will be linearly dependent on the probability of finding an As atom, i.e. the surface coverage.

The arsenic deposition rate was found to follow

$$d_{R} = \frac{260}{1 + e^{\frac{\theta - 0.1}{0.075}}} \operatorname{Torr}^{-1} \mathrm{s}^{-1}.$$
 (6)

The decrease of the deposition rate with As surface coverage is governed by the same physical principle as the decrease in the growth rate. It was already shown that As deposition stops after forming a full monolayer [9], and this form of the deposition rate was chosen according to the typically observed dependence of the sticking coefficient on coverage [8]. In Fig. 2 expected doping profiles assuming a constant deposition rate, and a deposition rate according to (6), are plotted.

The incorporation rate was found to depend on the arsine partial pressure as

$$i_R = 1 \cdot 10^{-4} + P_{A_S} \cdot 20 \text{ Torr}^{-1}.$$
 (7)

The constant term corresponds to the probability of an As atom not segregating. As we have not observed the dependence of the incorporation rate on the growth rate, we can conclude that this probability represents the equilibrium probability. This means that the segregated state is energetically approximately 0.85 eV more favourable. The term proportional to the arsine partial pressure can be justified by noting that if during epi growth and As deposition an As atom from the surface, which happens to be covered by another As atom, will have reduced probability of segregating. The influence of this term can be appreciated by plots such as shown in Fig. 3 where predicted doping profiles are compared when assuming either the constant incorporation rate (dashed lines) or the incorporation rate according to (7) (solid lines).

Limitations on profiles

The only fundamental limitation on the doping profile is the upper boundary set by the maximum coverage and maximum arsine partial pressure. We have not attempted to measure this value, and the presented model should not be ad hoc extrapolated.

All other limitations on the doping profiles can be circumvented with varying degrees of processing complications. The second most significant limitation is on the creation of



Fig. 1. C-V doping profile (dots) of a sample grown at 800 °C with gas flows of H_2 50 slm and dichlorsilane 296 sccm. The solid line gives the "true" profile as assumed from the combined knowledge of the method of growth and the C-V profile. The sharp increase in doping at 1.17 um corresponds to the initial pure As deposition. The exponential decrease in doping is due to As incorporation from the As surface coverage layer during the subsequent Si epi growth. The non-abrupt appearance of the C-V profile is due to electron out-diffusion as was confirmed by MEDICI simulations. Correcting the C-V profile for electron diffusion gives a good fit to the solid line.



Fig. 2. Samples grown with constant arsine partial pressure. Aggregated results of 12 C-V profiles (dots), expected doping profile according to the presented model (solid line) and the expected doping profile assuming a deposition rate independent of coverage (dashed line).



b)

Fig. 3. (a) and (b) show two different doping profiles grown with increasing arsine partial pressure at 800 °C, with gas flows of H_2 50 slm and dichlorsilane 296 sccm. The dots indicate the segmented C-V profiles, the solid lines the doping profiles predicted by the new model and the dashed lines the doping profiles predicted by assuming an incorporation rate independent of the arsine partial pressure. In (b) a spread of the C-V profile due to imperfect bake-off and electron diffusion is visible.

a sharply decreasing profile. The characteristic length of the doping profile when As is not being deposited is in the order of 1500 nm. Therefore a sharp drop in doping can be achieved only by baking off arsenic by heating up the sample until desorption becomes significant. However, increasing the temperature above 900°C would cause undesired As diffusion, and perfect bake off is difficult to achieve within a reasonable time.

Finally, the upper and the lower boundary of the partial pressure of arsine may appear as limitations on creating very abruptly increasing or very slowly changing doping profiles. These, however, can be easily circumvented by adding processing steps in which only As is being deposited or no As is being deposited.

CONCLUSION

It has been demonstrated that the proposed model for As dopant incorporation during Si RPCVD epitaxy gives much better predictions of the as-grown doping profiles than previous, more simplistic, models. The epitaxy process was characterized to obtain functional dependencies of the parameters that are important for describing the processing conditions. This enabled us to have unequalled control over the shape of the doping profile.

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