Interdiffusion at Ge/Si Interfaces Studied with AES Depth Profiling

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Interdiffusion at the interfaces of a multilayer structure consisting of 3 Ge layers of about 2.2, 4.3 and 2.2 nm thickness in a Si matrix was studied by depth profiling with AES. Measured depth profiles of the as deposited structure (grown at 300° C), taking the Ge LMM peak intensity as a function of the sputtering time, were compared with those obtained after annealing of the sample at 600, 650, and 700°C after quantitative evaluation with the MRI (mixing-roughness-information depth)-model. As a result, the interdiffusion constant was determined (D_{eff} = 6.3 E-22 m^2/s at 973 K) as well as the activation energy (E ≈ 0.9 eV). These values are considerably lower than the bulk diffusion coefficients. This effect presumably is connected with the strain in thin film multilayer Si/Ge heterostructures due to the lattice mismatch. It is especially important at low temperature annealing and has to be taken into account in the fabrication technology of of Si/Ge nanostructures.

Introduction

Strained Ge/Si heterostructures grown by molecular beam epitaxy (MBE) have attracted interest because of their applications to many microelectronic and optoelectronic devices such as heterobipolar transistors, infrared photodetectors, optical waveguide devices etc. In all these applications, the abruptness of Ge/Si interfaces have a great significance. The heat treatment processes that inevitable presents in device fabrication processes may lead to atomic interdiffusion in interfacial region.

The aim of the present work is to study the post growth annealing behavior of multilayer Ge/Si structure grown at low temperature.

Experimental

Sample preparation.

The original structures were grown using a MBE installation "Katun-C" equipped with two e-beam evaporators for germanium and silicon and two Knudsen cells for doping and RHEED system for growth process control. Germanium silicon films were grown on p^+ Si(001) substrates. Each silicon layer was doped by delta-layer of B of a concentration of $6x10^{11}$ cm^{-2}. The as grown structures consisted of the following prospective layers (in direction of growth from the Si(001) substrate:

- Si buffer layer of thickness 55 nm (Temperature of growth T=800°C)
- Ge layer of equivalent thickness 1.4 nm (T=300°C)
- Si layer of thickness 5 nm (T=500°C)
- $Ge_{0.4}Si_{0.6}$ layer of thickness 4 nm (T=500°C)
- Si layer of thickness 5 nm (T=500°C)
- Ge layer of equivalent thickness 1.4 nm (T=300°C)
- Si layer of thickness 55 nm (T=500°C)

Prior each Ge layer growth the growth process was interrupted and the growth temperature was lowered to T=300°C to eliminate interdiffusion.

Post growth annealing of samples was done in argon ambient during 30 minutes per each temperature (600, 650 and 700°C).

AES Depth Profiling.

Experimental investigations were conducted in a Surface Science Center (Riber, France) with CMA energy analyzer OPC-200 and coaxial electron gun.

Measurements were carried out in the derivative mode with a modulation voltage of 4 V. The AES conditions were as follows: primary electron beam energy 5 keV, beam current 100 nA, beam diameter about 3-5 μm, electron beam incidence normal to the surface. The electron beam was rastered over a region of 15 x 20 μm. Sputtering by Ar$^+$ ions was performed by using a CI-40 (RIBER, France) ion gun with angle of incidence equal to 74° to the normal to the sample surface. The ion etching conditions were as follows: ion energy 1.5 keV or 3 keV, Ar gas pressure 2x10^{-5} Torr, ion current 200-400 nA, ion beam diameter about 0.9 mm. The ion beam was rastered over a region of 0.4 x 0.3 mm. AES measurements were done between the sputtering cycles.

MRI calculations:

The reconstruction of the original in depth distribution of composition was made using the MRI-model [1,2], based on a quantitative description of the effects of ion sputtering and analysis method.

Results and Discussion

Figure 1 shows the measured Ge profile together with MRI fitting after quantification of the AES intensity and the fitting procedure described in [3] for the "as grown" sample. The optimized fit, corresponding to TEM investigations, shows a reduced Ge concentration of $X/X_0 = 0.6$ (prospective value 1.0) for layers 1,3 and $X/X_0 = 0.37$ (nominally 0.4) for layer 2. The thickness of layers 1,3 was found to be 2.16 nm instead of the prospective value of 1.4 nm. This result is in good correlation with TEM study of low temperature thin Ge layer on Si [4].

The results of depth profiling and the corresponding MRI fitting for samples after annealing at 600, and 700°C are presented on Figs. 2 and 3. It is obvious that that the

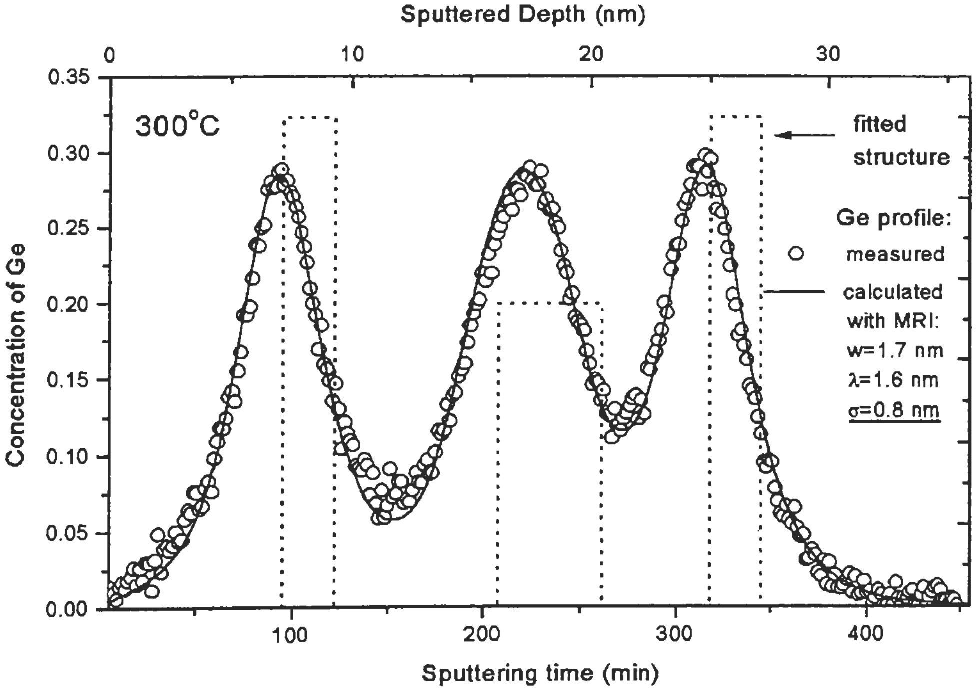

Fig. 1: Measured Ge depth profile, Calculated MRI profile and reconstructed original in depth distribution (fitted structure, right conc. scale (0... 0.65)) for the "as grown" sample.

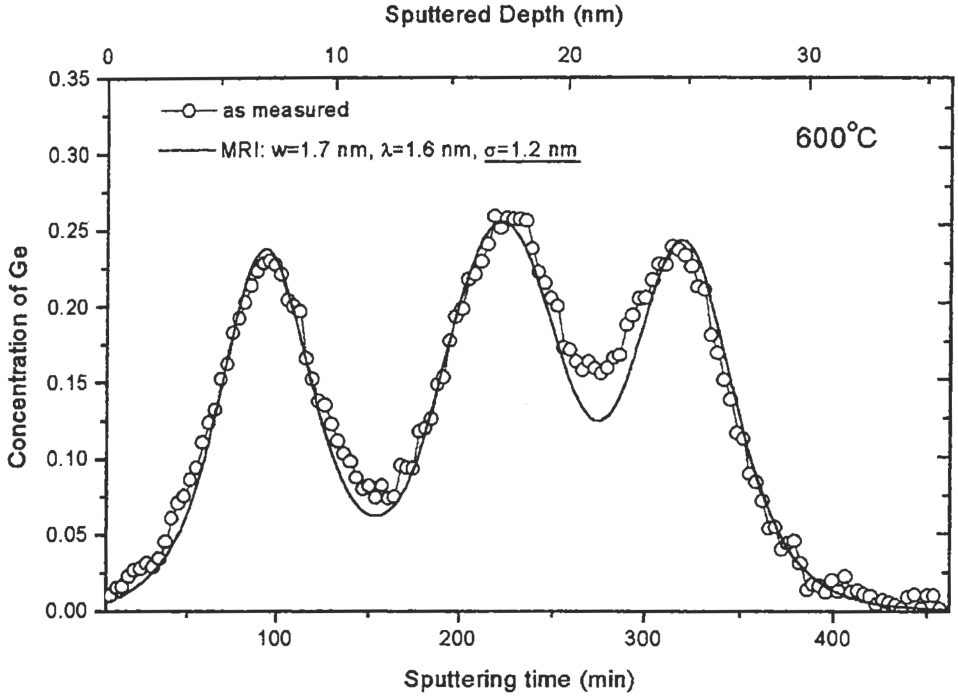

Fig. 2: Ge depth profile of the structure of Fig. 1, after annealing at 600°C (30 min) and profile fitting with the MRI-model. Note that only σ is changed as compared to Figs. 1and 3.

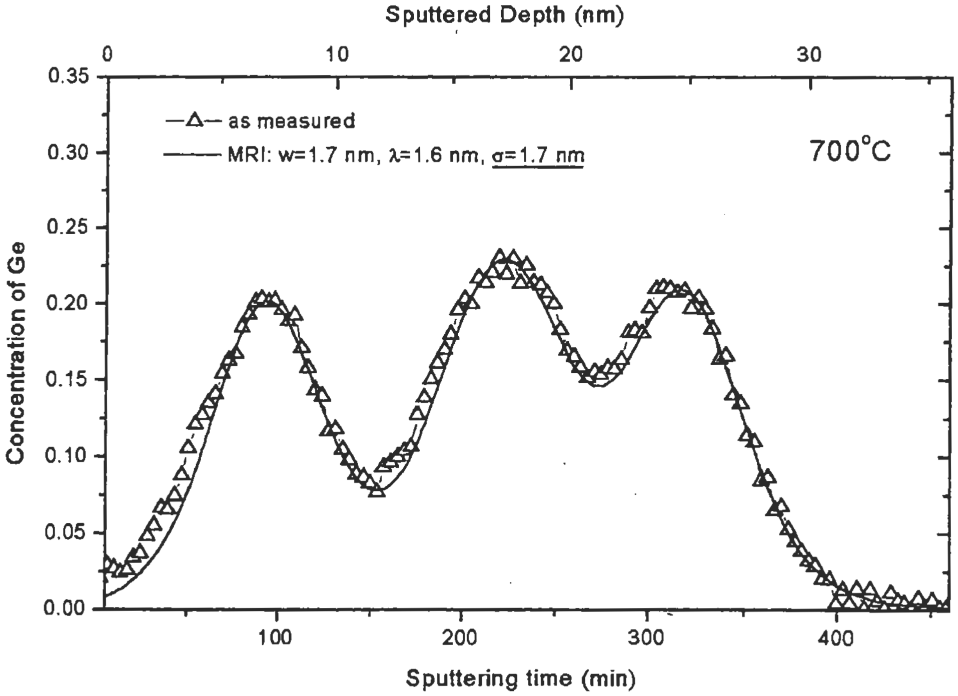

Fig. 3: Ge depth profile of the structure of Fig. 1, after annealing at 700°C (30 min) and and profile fitting with the MRI-model. Note that only σ is changed as compared to Figs. 1and 2.

annealing already at 600°C results in profile broadening and in a visible decrease of the Ge LMM intensity of layers 1 and 3. For simplicity, we treat here the Ge/Si interdiffusion as ideal tracer diffusion with Gaussian broadening of ideally sharp interfaces, using the Gaussian MRI parameter σ as a measure of the interdiffusion constant D_{eff} and the relation:

$$2tD_{eff} = \sigma^2_{Diff} = \sigma^2_T - \sigma^2_0 \qquad (1)$$

with σ_T and σ_0 the σ parameter after annealing at temperature T and without annealing, respectively (see inset in Figs.1-3). The results of the calculations of the interdiffusion constant after eqn. (1) are shown in the Arrhenius plot in Fig.4.

As seen already in the "as grown" (300° C) data and in the following profiles after annealing, some matter between the layers is not well represented and /or the diffusion coefficient is higher for lower Ge concentrations.

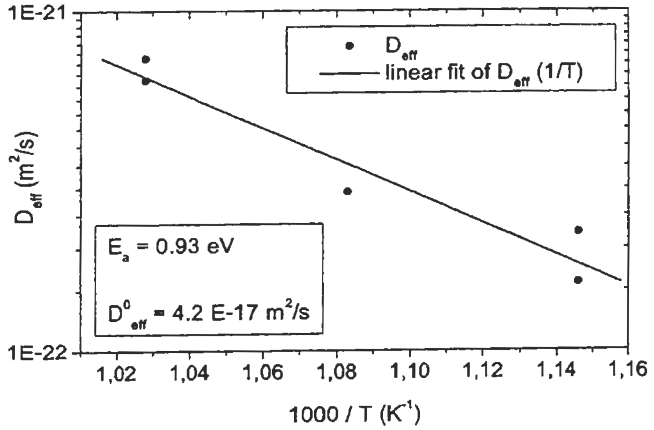

Fig. 4: Arrhenius plot of the D_{eff} values from eqn. (1).

The interdiffusion constant determined from Fig. 4 ($D = 4.2\times10^{-17}\times \exp(-0.93/kT)$ m²/s) shows a considerably lower preexponential term (D^0_{eff}) and activation energy ($E_a = 0.93$ eV) as compared to the bulk diffusion coefficients measured in [5] ($D^0_{eff} = 4.5\times10^{-8}$ m²/s, $E_a \approx 3$ eV) , but they are in good accordance with the results of other works: [6] - concerning the investigation of strain-induced diffusion in a strained $Si_{1-x}Ge_x$ / Si heterostructures by TEM and [7] - direct observation of intermixing at Ge/Si(001) interface during annealing at 300-800°C by HRRBS.

Conclusion

We have shown that AES depth profiling provides direct observation and, in combination with the MRI model, quantitative determination of the strain-enhanced diffusion in thin film multilayer Si/Ge heterostructures. This effect is especially important at low temperature annealing and has to be taken into account in the fabrication technology of of Si/Ge nanostructures.

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