



Experiment title:
**In-situ characterization of recrystallization kinetics
of a-SiGe structures**

**Experiment
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HS-2

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Report:

Previously, we studied the amorphous SiGe crystallization in both doped and undoped SiGe films by in-situ TEM and ex-situ XRD. Both techniques suffer of certain disadvantages to describe the crystallization process in general: in-situ TEM needs extra precautions to avoid e-beam heating and radiation damage influencing crystallization, and thus it is only able to characterize accurate the incubation time t_0 , the grain growth rate, and the grain size in any moment of crystallization. Ex-situ XRD is useful to characterize crystalline SiGe spacing. Therefore, we utilized the unique in-situ XRD method for general description of the Random Nucleation and Growth (RNG) process in amorphous SiGe and to demonstrate doping effects on crystallization.

We investigated undoped and B-doped $\text{Si}_{1-x}\text{Ge}_x$ films, 0.2 μm thick with compositions $x = 0, 0.25, 0.5, 0.75,$ and 1, which were deposited by molecular beam on $\text{SiO}_2/\text{Si}(001)$ substrates at a temperature of 200°C. Θ - 2Θ scans of the (220) reflection were measured to follow the crystallization process in high vacuum ($< 10^{-6}$ Torr) in the temperature range from 300 to 1000°C for 15 min to 12 h. The energy of the x-ray beam was 7.58 keV.

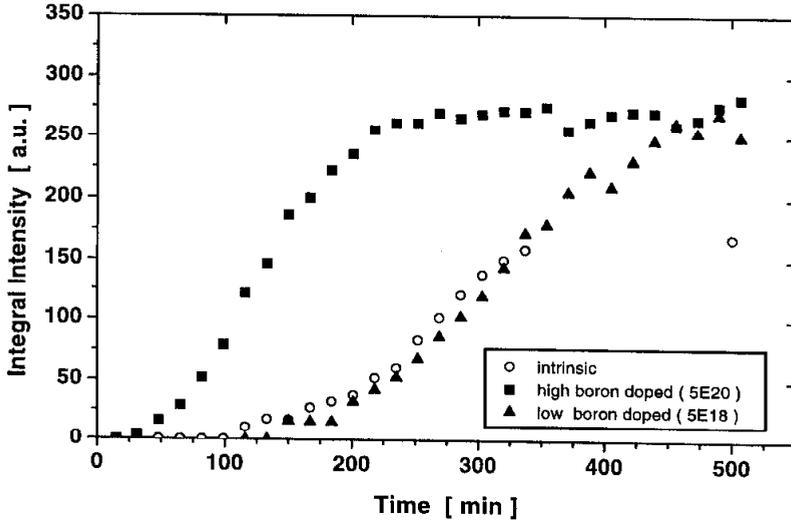
The measurements enabled us to follow the crystallization process from its onset until completeness by determination of the integral intensity of the (220) peak of the crystallized SiGe. Since the integrated intensity is proportional to the crystalline fraction in the film, its

time dependence under isothermal annealing should be described by the formula

$$f(t) = 1 - \exp[-(t-t_0)/\tau]^n, \quad (1)$$

where t_0 is the incubation time for crystallization, τ the time for a crystallization fraction $(1 - 1/e)$, and n describes the kind of crystallization ($3 \leq n \leq 4$ for 3-dimensional and $2 \leq n \leq 3$ for 2-dimensional transformation).

The figure shows as an example experimental data of isothermal anneals at 550°C for both undoped and doped $\text{Si}_{1.5}\text{Ge}_{0.5}$ films.



The conclusion from our in-situ XRD results is that the doping level affects the crystallization process in a similar way as with raising annealing temperature - the transformation is accelerated by a high concentration of Boron in the $\text{Si}_{1.5}\text{Ge}_{0.5}$ films.

All experimental curves could be well-described by formula 1, and characteristic parameters were obtained for a set of different samples at different temperatures.

Another interesting effect of doping which was detected by in-situ XRD experiments is the variation of lattice parameter with dopant concentration. The experimental values show a reduction of the lattice parameter by 0.65 % for a B concentration of $5 \times 10^{20} \text{ cm}^{-3}$ and of 0.21% for a concentration of $5 \times 10^{18} \text{ cm}^{-3}$, compared to the lattice parameter of the undoped sample. These values are surprisingly large, especially for the case of lower B concentration, compared to values calculated according to Vegard's law. The reason for this evident decrease in lattice parameter may be the result of compressive stresses in the crystalline phase in the case of the doped samples, or the result of a change in the composition (x) of the crystalline phase. The solubility of B in the alloy $\text{Si}_{1-x}\text{Ge}_x$ is not known. It was found that the undoped samples crystallize with a relatively unchanged lattice parameter, while the lattice parameter of the doped samples decreases during the crystallization process. This could be the result of developing stresses or variation of composition (x) in the crystalline phase.