ESRF	Experiment title: In-situ study of the crystallization kinetics of undoped and doped amorphous SiGe films	Experiment number: HS-454
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Report:

Modern thermoelectrical devices as well as the technology of Active-Matrix Liquid Crystal Displays need materials for the fabrication of thin film transistors on glass or other insulating and flexible substrates. Polycrystalline $Si_{1-x}Ge_x$ is known as a prospective one due to its (i) high mobility, (ii) lower than for amorphous Si crystallization budget, and (iii) low dopant activation barrier. The solid-phase crystallization (SPC) process to transform originally amorphous $Si_{1-x}Ge_x$ film to crystalline is preferable because of its flexibility to regulate the grain size.

Previously (ESRF experiment HS-2), we studied the amorphous SiGe crystallization of undoped and B-doped $Si_{1-x}Ge_x$ films, 0.2 µm thick with compositions x = 0, 0.25, 0.5, 0.75, and 1, which were deposited by molecular beam on $SiO_2/Si(001)$ substrates. The aim of this experiment (HS-454) was to extend the crystallization studies to phosphorous doped $Si_{1-x}Ge_x$ films with different Ge content, since only the combination of p-doped and n-doped materials allows the fabrication of many thermoelectric devices etc.

Due to some beamline problems (necessary replacement of the beamline monochromator, new adjustment etc.) and the following reduction of measuring time we had to concentrate our studies to films with 50% Ge concentration $(Si_{0.5}Ge_{0.5})$ and different P-doping levels.

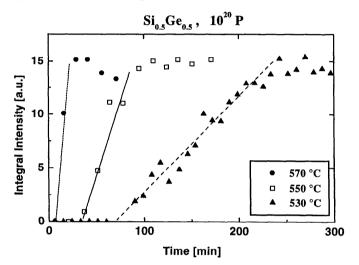
O-20 scans of the (220) reflection were measured to follow the crystallization process in high vacuum ($<10^{-6}$ Torr) in the temperature range from 500 to 600°C.

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 can be described by the formula

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

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

The figure shows as an example experimental data of isothermal anneals at 530°C, 550°C, and 570°C for highly $(10^{20} \text{ cm}^{-3})$ P-doped Si_{0.5}Ge_{0.5} films.



All experimental curves could be well-described by formula 1. The characteristic crystallization data (t,, τ , and n) were obtained for two different P-doping levels (10^{20} and 10^{18} Pcm⁻³) of Si_{0.5}Ge_{0.5} films in their dependence on the temperature.

In conclusion of both experiments (HS-2 and HS-454), the crystallization kinetics of undoped and doped (by boron and phosphorous) $Si_{1-x}Ge_x$ films was investigated in detail by in-situ XRD. The Si/Ge ratio in the film, together with the B and the P concentration determine the rate of the transformation from amorphous to crystalline state, so that together with the suitable annealing regime the resulting film microstructure can be controlled.