Optical-structural correlation of $fesi_2$ nanoparticles produced by ion-beam-induced epitaxial crystallization in fe^+ implanted sio_2/si followed by thermal annealing

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Metallic and semiconducting silicides are of significant interest for silicon-based technologies. The $FeSi_2$ is the unique transition-metal silicide that owns a semiconducting (β) and two distinct metallic phases (α and γ). In particular, β-$FeSi_2$ has been recognized as a promising material for applications in optical devices due to its photoresponse properties in the NIR region at 1.55 μm.

We have synthesized and investigated the optical-structural correlation of $FeSi_2$ nanoparticles produced by ion-beam-induced epitaxial crystallization (IBIEC) in Fe^+ implanted SiO_2/Si(100) substrate followed by thermal annealing. For this, Fe^+ ions were implanted at cryogenic temperature (– 180 °C) in two steps: i) 70 keV at the fluence of $5x10^{15}$ cm^{-2} and ii) 40 keV at the fluence of $3x10^{15}$ cm^{-2}. Such implantation produces an amorphous Si layer that subsequently was recrystallized under high-energy irradiation using a 600 keV Si^+ beam with the substrate at 350 °C.

Rutherford Backscattering Spectrometry combined with ion Channeling Technique was used to monitor the IBIEC process and evaluate the structural quality of the samples. The formation and phase transition were identified by Micro-Raman Scattering Spectroscopy. Transmission Electron Microscopy images allowed revealing the phase morphology. The results show that the IBIEC process leads to an efficient amorphous layer regrowth and the nucleation of two types of γ-$FeSi_2$ nanoparticles: spherical (A-type) and plate-like (B-type). After annealing at 700 °C/1h, it was observed an A-type to B-type evolution and formation of hemispherical-like β-$FeSi_2$ nanoparticles at the SiO_2/Si interface. Upon thermal treatment at 800 °C/1h, there was a complete phase transition from γ to β.

Photoluminescence measurements at 2 K showed only excitonic complex emissions from Si substrate in the as-recrystallized sample. After annealing, a broadband emission centered at 0.79 eV is observed in the spectra assigned to optical transition from β-$FeSi_2$.