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Ion-induced epitaxy in Fe^+ implanted SiO_2/Si: synthesis and optical characterization of $FeSi_2$ nanoparticles

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Abstract – $FeSi_2$ nanoparticles have been synthesized by ion-beam-induced epitaxial crystallization (IBIEC) of Fe^+ implanted SiO_2/Si(100) followed by thermal treatment. As evaluated by Micro-Raman scattering spectroscopy and Transmission Electron Microscopy, upon annealing at 700 °C / 1h occurs a transition from metallic γ to semiconductor β phase in the recrystallized sample (Fig. 1). Photoluminescence spectroscopy measurements at 2K revealed strong emissions with different intensities and morphologies in the region 0.7 - 1.1 eV (Fig. 2). The physical origins of the distinct luminescence peaks were discriminated in terms of intrinsic emission of β-$FeSi_2$, optically active defect-centers in Si and intrinsic substrate emissions (excitonic complex).

Semiconducting silicides are of significant interest for silicon-based optoelectronics, optical interconnects and optical communications technologies. Among the transition-metal silicides, $FeSi_2$ is the unique that owns a semiconducting phase (β) and two distinct metallic phases (α and γ). In particular, the semiconducting β-$FeSi_2$ is a promising material for photodetectors, light emitters and solar cells devices, due to value of the energy gap, which gives rise to photoresponse in the near-infrared region at about 1.55 μm.

We have synthesized and investigated the optical properties of $FeSi_2$ nanoparticles produced by ion-beam-induced epitaxial crystallization (IBIEC) in SiO_2/Si(100) n-type substrates. For this, Fe^+ ions were implanted at cryogenic temperature (~ 90 K) 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}. This implantation process produces an amorphous silicon layer of ≈ 115 nm thickness that was subsequently recrystallized by high energy irradiation with Si^+ ions at 600 keV with the target at 350 °C.

By Micro-Raman Scattering Spectroscopy (μRSS) we have identified the vibrational properties and thermal stability of the distinct $FeSi_2$ phases. Moreover, we show that annealing at T = 700 °C / 1h (in a gas atmosphere 95% N_2 - 5% H_2) leads to complete phase transition from the metastable γ to the β phase. Our Transmission Electron Microscopy (TEM) results corroborate the μRSS characterization.

Photoluminescence (PL) measurements at 2 K showed only excitonic complex emissions from Si substrate in the as-IBIEC sample. After 700 °C annealing, a broad band appearing at ~ 0.79 eV can be attributed the intrinsic emission from β-$FeSi_2$. However, optical absorption spectra (300 K) near the fundamental absorption edge of β-$FeSi_2$ indicated indirect allowed transition. A phonon structure corresponding to the emission and absorption component was clearly observed.

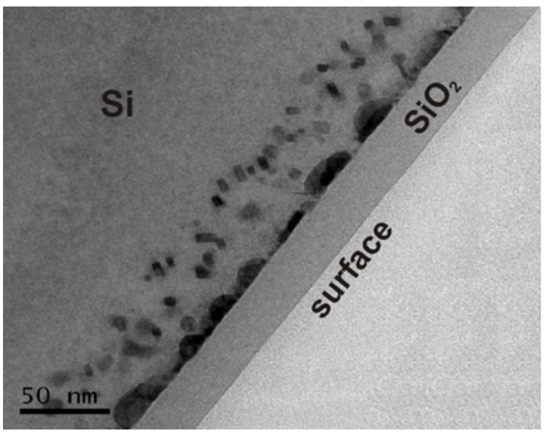

Figure 1: Cross section TEM image (700 °C annealed sample) showing the β-$FeSi_2$ precipitates close to the SiO_2/Si interface within the Si matrix.

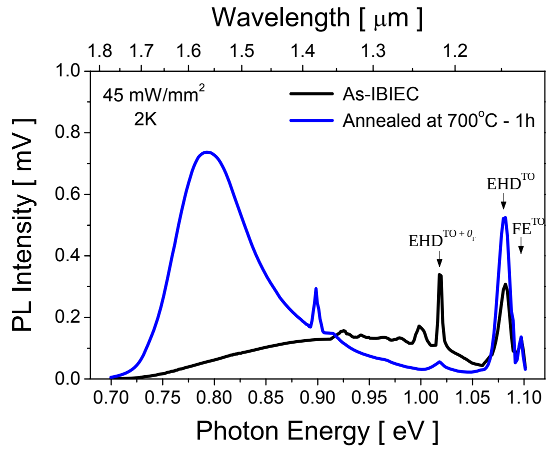

Figure 2: PL spectra (at 2 K) presented a prominent band at ~ 0.79 eV (700 °C annealed sample) beyond of excitonic complex emissions from Si substrate (also observed in the as-IBIEC sample).