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The effect of ion implantation energy and dosage on the microstructure of the ion beam synthesized $FeSi_2$ in Si

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Abstract

Nanometer-sized β-$FeSi_2$ precipitates are formed in Si by ion beam synthesis (IBS). A systematic study is carried out to investigate the correlation among the implantation parameters, the microstructure, and the luminescence properties. On the one hand, we found additional orientation relationships (ORs) appear between the β-$FeSi_2$ and the Si with improved lattice coherence between the two, when the ion implantation energy is increased. On the other hand, the degree of preferential orientation deteriorates and leads to poor lattice coherence between the particles and Si matrix when the iron ion is overdosed. These microstructure changes lead to different luminescence properties (intensity, peak position and shape) of the β-$FeSi_2$ particles accordingly.

Keywords: Ion implantation energy; Semiconducting β-$FeSi_2$; Ion beam synthesis

1. Introduction

Semiconducting β-$FeSi_2$ has orthorhombic structure with lattice constants of $a = 0.9863$ nm, $b = 0.7791$ nm, $c = 0.7833$ nm [1]. The band gap of the material is reported to be ∼0.8 eV (corresponds to a wavelength of 1.55 μm), matching the preferred wavelength window for optical communication systems [2–3]. Together with its promising optical properties, the convenience of incorporating $FeSi_2$ into the current Si-based microelectronics for photonic applications has attracted great research attention in the past decade. Various techniques have been employed to prepare β-$FeSi_2$, such as pulsed laser deposition (PLD) [4], reactive deposition epitaxy (RDE) [5], molecular beam epitaxy (MBE) [6], and ion beam assisted deposition (IBAD) [7]. Among them, ion beam synthesis (IBS) is one of the most widely used techniques and is capable of producing samples with $FeSi_2$-particle/Si-matrix configuration, in which the β-$FeSi_2$ phase serves as effective light emitting materials [8–10].

Various processing parameters of IBS play important roles in determining the microstructure of $FeSi_2$ such as phase, lattice coherence with the Si matrix, and strain, etc. which further affect its luminescence properties. In fact, several orientation relations between the $FeSi_2$ and the Si have been identified experimentally, and the correlations between the specific microstructure and luminescence properties of the material have been elaborated. For example, Maeda et al. showed that better interfacial structure between the β-$FeSi_2$ precipitates and the Si would enhance the photoluminescence (PL) intensity [11], Spinella and co-workers showed that the large unstrained β-$FeSi_2$ precipitates give the PL signal at 1.54 μm [10]. On the other hand, it has also been theoretically predicted that the presence of suitable strain changes the β-$FeSi_2$ band gap value as well as its nature from indirect to direct [12–13]. Unfortunately, the available literature results are both limited and scattered. In many cases, discrepancies exist among individual works. Therefore, a systematic study to investigate the correlation among the implantation parameters, the microstructure and the luminescence properties is needed, in order to understand the fundamental physics that govern the luminescence properties of the $FeSi_2$, which would further guide the engineering process of this promising photonic material.

In this work, $FeSi_2$ precipitates are formed in Si using IBS with two series of systematically designed processing parameters. The microstructures of the resulted $FeSi_2$ precipitates were

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investigated using transmission electron microscopy (TEM), and the corresponding photoluminescence properties were examined. The effect of ion implantation energy and dosage on the microstructure evolution and the luminescence properties of the β-$FeSi_2$ particles are discussed.

2. Experimental

The samples were prepared using iron ion implantation into (1 0 0) p-Si wafer (resistivity ∼15–25 Ωcm) using a metal vapor vacuum arc (MEVVA) ion source. In order to investigate the effects of both the implantation energy and the ion dosage on the microstructure and the luminescence properties of the samples independently, we designed two experiment series. In the implantation energy series, the three samples, which are referred to EN1, EN2, and EN3, were implanted at extraction voltages of 40 kV, 60 kV, and 80 kV, respectively, at a fixed total dose of 5×10^{15} ions/cm^2. In the dosage series, the extraction voltage was kept fixed at 80 kV with three different doses of 1×10^{15}, 5×10^{15} and 1×10^{16} ions/cm^2, for the samples DO1, DO2, and DO3, respectively. The implantation temperature was maintained at approximately −100 °C for all the samples so that a dislocation-free layer would be expected after annealing according to a previous report on the study of implantation temperature effect [14]. The as-implanted samples were then subjected to a dual step annealing process, i.e. firstly annealed using a rapid thermal annealing (RTA) at 850 °C for 20 s, followed by a furnace annealing (FA) at 850 °C for 10 h. The microstructure characterizations of the annealed samples were carried out using transmission electron microscopy (Philips CM120, and Tecnai 20 ST). The detailed phase identification and orientation relation between the Fe–Si phase and the Si matrix were examined using transmission electron diffraction (TED). The luminescence properties of the annealed samples were studied by photoluminescence (PL), which were performed at 80 K using the 514 nm line of an argon laser with a power of 150 mW as the excitation source. The light emission was dispersed using a1 m monochromator and detected by a liquid nitrogen cooled Ge detector.

3. Results

The TEM results of the as-implanted samples (not shown here) revealed that an amorphous layer of Fe–Si mixtures was formed on top of the crystalline Si. The thickness of the layer is determined by the implantation parameters such as ion energy and ion dosage. The iron silicide phase would precipitate out only after the annealing process.

3.1. Ion energy series

$FeSi_2$ particles of similar sizes are formed in sample EN1, EN2, and EN3 after annealing. The selected area electron diffraction patterns (SADP) taken from their planview TEM samples are shown in Fig. 1(a)–(c), respectively. The SADPs were taken with the electron beam parallel to the Si [1 0 0] zone axis. Extra diffraction spots not belonging to Si are observed (as marked by arrows). In order to identify the phase origin of these extra diffraction spots, micro-diffractions (μ-diffraction) are taken from the particles that give the specific diffractions as marked by arrow d–f in Fig. 1(a)–(c), respectively. All of the μ-diffractions (Fig. 1(d)–(f)) can be indexed to the orthorhombic β-$FeSi_2$ phase (S.G: Cmca (64)) [1,15] but having different orientation relationships (OR) with the Si matrix.

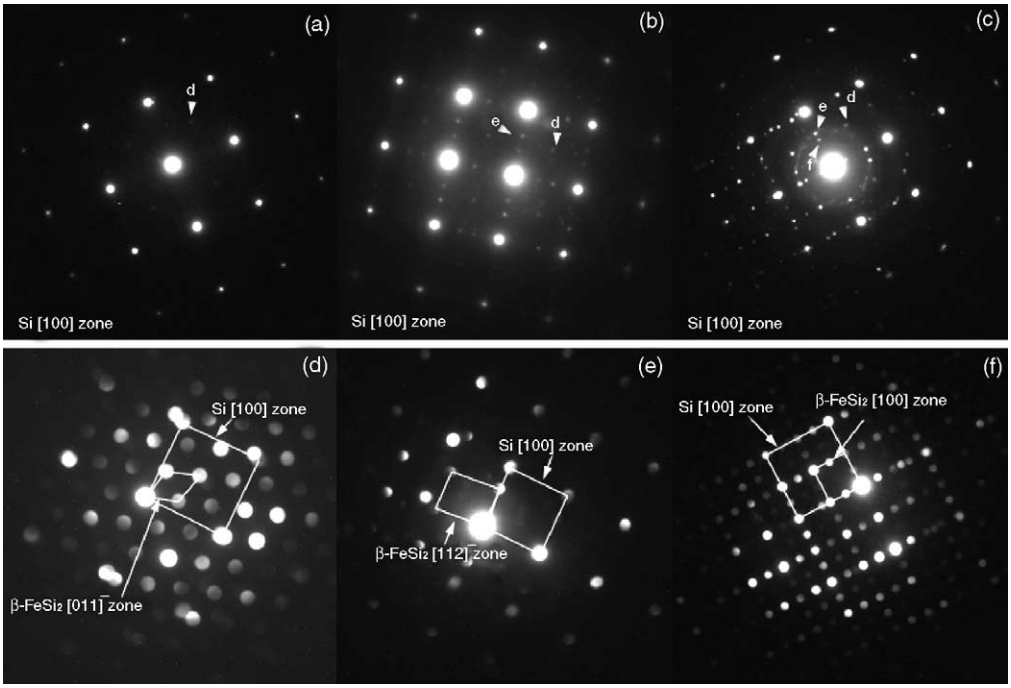

Fig. 1. (a)–(c) are the SADPs taken from planview EN1, EN2 and EN3 respectively; (d)–(f) are the μ-diffraction patterns taken from the particles corresponding to the specific diffraction spots as marked by arrows d–f in (a)–(c), respectively.