



Formation mechanism of NdSi₃N₅ nanocrystals via hot-injection and heat-up methods

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ABSTRACT

NdSi₃N₅ nanoparticles were successfully synthesized and stabilized with hot injection and heat up methods. We have, therefore, investigated the influence of the heating time (ta) variation to study the film morphology, structural and optical properties. Deep demonstrations based on X-ray diffraction, Raman spectroscopy, X-ray fluorescence analysis and Fourier transform infrared spectroscopy reveal the formation of the expectant NdSi₃N₅ compound for optoelectronic devices. The results showed that phase separation occurs during the annealing process due to the condensation of the Si excess; bring about in orthorhombic phase stability. Basing on bonds confinement model, the result of Raman spectroscopy has surprisingly revealed an important property of nano-structuration behavior as detected by high-resolution scanning electron microscopy. The resulting material has interesting physical properties, which are sought after in many optoelectronic industries.

1. Introduction

Silicon nitride has attracted interest in several technology applications as mechanical, resistance to oxidation, thermal shock, optoelectronics, and photovoltaic industry [1–3]. The Si₃N₄ exists in two stable hexagonal polymorphs (designated α[P31c]- and β[P6₃/m]-Si₃N₄) with very similar structures [4] both being obtained under conventional conditions. The α-Si₃N₄ phase is built basing on SiN₄ tetrahedrons and can irreversibly transform into β-Si₃N₄ at high temperatures, which is twice as short. Despite being cheap, these crystalline structures and their nanostructuration advance solar cell technology as an emerging topic of research in the photovoltaic field due to the efficient light absorption. Therefore, light trapping schemes must be developed to increase the efficiency of solar cells based not only on the film nanostructuration but also on the type and the addition of a rare-earth (RE) ions amount, which can improve the optoelectronic properties and can show relatively lower barrier for carriers within more intense light emission [5,6]. Likewise, the silicon nanoparticles (Si-NPS) act as efficient energy sensitizers for rare-earth (RE) ions incorporation [7] causing a shift of the emissions for

a wider photon energy range [8]. An earlier study has been accomplished using a mixture of Nd₂O₃ with silicon-rich silicon nitride (SRSN) compounds as active materials, taking advantage of the superior optoelectronic performance provided by Si-NPs [9]. Further Si-NPs have a smaller size [10]; this is advantaged to separate the oxygen from Nd₂O₃ clusters, which caused a quench of Nd³⁺ emitting-light [11]. In this situation, the Nd concentration should be small so that full-color luminescence being intense [12].

However, the silicon nitride material has a breakdown strength of 9 MV/cm [13] and a bandgap of 5.3 eV leading sufficiently to confine the charge carriers in the lattice (versus to 9 eV as band gap of SiO₂) [14,15]. Although the nature of bandgap changes from indirect to quasi-direct due to the decrease in grain size, in that case, the room temperature photoluminescence (PL) can have an intense emission in the visible range [16]. Further, the Si-NPs were grown and formed clusters with Nd³⁺ ions; they lead to an increase in the Nd³⁺ energy sensitizer and allowing one to obtain high content of Nd³⁺ ions sensitized, which is the key parameter to achieve future photonic components [17]. Kenyon et al. [18] demonstrated that the presence of Si-NPs exhibits an increase in

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