PHOTOLUMINESCENCE AS A SURFACE-EFFECT IN NANOSTRUCTURES

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Abstract — Nanocrystalline Si powder prepared by Laser Induced CVD (LCVD) showed photoluminescence (PL) at wavelengths of 400-900 nm when excited at 488 nm and 330 nm. The powder consists of spherical grains with an average diameter of 25 nm and log-normal size distribution. In this study we present a model which explains the origin of the photoluminescence: the latter is generated by electrons which jump from the regular bulk-states into the sulfate-states of the nanocrystals, which in turn are not populated after being excited by the illuminating photons. We present the effect of the surface potential on the surface states and, thus, on the possible transitions. The model is tested against experimental results which cannot be explained by the quantum size confinement effect such as photoluminescence from particles bigger than 10 nm and shift in the PL emission wavelength due to oxygen and nitrogen bonds at the surface of the particles. The tools presented here can be applied also to porous silicon.

1. INTRODUCTION

Visible photoluminescence (PL) with a few percent quantum efficiency was observed in porous silicon at room temperature and was first reported in 1990 (1); the porous Si layer contains Si crystallites with a typical size of 2-5 nm (2). Photoluminescence, similar to that of porous Si (PS), has also been observed in clusters of nanosized grains (3-5). The great interest in this phenomena originates from its potential application in light emitting devices based on well-known silicon technology. Application of PL to Si-based devices requires an understanding of its mechanism and its dependence on microstructure and composition. Two main models have been proposed to explain PL in porous Si: (i) physical quantum size confinement effect, and (ii) chemical quantum size confinement effect; however, there are various experimental results which cannot be accounted for by either.

The most frequently quoted mechanism is the physical quantum confinement of electrons in nanometer size crystallites (2,6,7), in spite of the fact that no direct evidence for discrete quantum confinement levels has been demonstrated to date. According to this model, quantum confinement in fine silicon structures can lead to symmetry-allowed optical transitions across the gap with an energy in the visible range. In other words, the nanocrystals have a direct gap which