Trapping Phenomena in Nanocrystalline Semiconductors

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Trapping phenomena play an important role in electrical and optical behavior of the nanocrystalline semiconductors. While the trapping phenomena in bulk semiconductors are dominated by the traps located in the volume, in nanocrystals these phenomena are dominated by those located at the surface/interface. This is due to the very big area/volume ratio (more than 10^8 m^{-1} for nanocrystals). The main specific processes that lead to the surface/interface trap formation are: (i) adsorption, (ii) dangling bonds, and (iii) internal stress (induced by misfit). The most investigations of the traps in nanocrystals were performed on silicon-based materials and structures, using a large variety of experimental methods.

The nanocrystalline porous Si (nc-PS) presents both types of traps, bulk and surface ones. Fresh nc-PS films, as well as stabilized by oxidation ones, were investigated in sandwich configuration Al/c-Si/nc-PS/semitransparent Al. Optical Charging Spectroscopy (OCS) and Thermally Stimulated Depolarization Currents (TSDC) methods were used [1, 2]. The OCS method is a less known zero bias method. It consists in the charging of the traps at low temperature by illuminating the sample with a suitable wavelength, followed by the detrapping induced by heating in dark. Thus, the detrapped carriers move in the frozen-in electric field of the still trapped ones. This way, the discharge current is a quadratic form of the trap concentrations and therefore the method is more sensitive than the others. The experimental curve allows the determination of the activation energies of the trapping levels and the estimation of the trap concentrations. A model of the trapping-detrapping processes in OCS allowed us to find trap parameters that cannot be experimentally determined (e. g. trapping cross-sections and non-equilibrium carrier lifetimes) [3]. Five maxima and shoulders were experimentally evidenced by OCS on fresh films (Fig. 1, Ref. 3) and one more appeared on stabilized ones. Only the first three of them could be measured by TSDC. The model resolved the maximum 2 in two levels (2' and 2''), and proved that the maximum F is a false maximum (does not correspond to any trap level). At the same time, the first four levels (1, 2', 2'', and 3) were proved to be due to surface traps, while the last ones were due to bulk ones. This was also checked by a comparison between native and anodically oxidized samples [4], which proved that the traps were similarly affected.

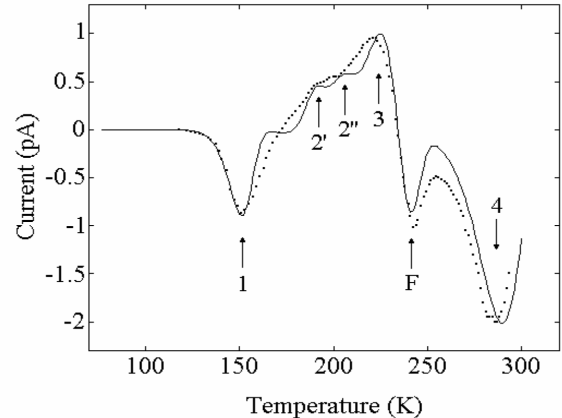

Fig. 1. Theoretical (continuous line) and experimental (dotted line) temperature dependence of the OCS discharge current for a fresh PS sample, polarized with $\lambda = 0.5$ µm [3].

A multilayer $(nc\text{-}Si/CaF_2)_{50}$ nanostructure was also investigated by both methods. The insulating properties of the CaF_2 obstruct the motions of the detrapped carriers (the tunneling current is at least 2 orders of magnitude smaller than the conduction one), so that part of them is retrapped. The TSDC measurements [5] showed a broad distribution of the activation energies, while the OCS ones [6] evidenced very sharp spikes, due to the dilatation misfit between nc-Si and CaF_2.

The traps found in nc-PS do not appear in the multilayer $(nc\text{-}Si/CaF_2)_{50}$ nanostructure (and reciprocally), because the interfaces are different (nc-Si/SiO_2 in nc-PS, and nc-Si/CaF_2 and nc-Si/nc-Si in $(nc\text{-}Si/CaF_2)_{50}$, respectively).

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