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Simulation of embedded nanocrystal effects on the electron beam induced current collected by a nano-electrode

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ABSTRACT

Three dimensional Monte-Carlo simulation is used to study the electron beam induced current technique. A circular and nanometric electrode is used to collect the induced current. This current is generated by the use of electron beam energy of 1 keV or 5 keV in a perpendicular configuration along a line passing through the electrode. The electrode – sample contact creates a depletion zone assumed of a hemispherical shape. The surface recombination velocity is assumed to be equal to zero, so each charge emerging at the surface of the sample can be collected with a given probability which depends on an opening angle allowing seeing the electrode. The collection process is affected by an embedded spherical nanocrystal which is considered as a recombination center. The strength of the effects depends on the depth of the nanocrystal and on the primary energy.

1. Introduction

For many decades, semiconductor low dimensional structures (nanocrystals, quantum dots, nano-wires,…) are widely studied for their specific properties, and promising applications [1–8]. Since their characterization needs new techniques to be able to help understanding their electronic and opto-electronic performances different techniques have been developed [9–12]. The electron beam induced current (EBIC) technique, by the use of a nano-electrode, is very suitable to study nano-materials. Indeed, collection of the electronic current by a conducting electrode which forms a nano-contact with the sample under test has been revealed as an interesting technique to characterize samples containing nanocrystals (NCs) [13–16]. The previous studies highlight a very high resolution of the technique which is called nano-EBIC. The nano-EBIC technique is also used to measure some physical parameters such as the minority carrier diffusion length (L_D) in the presence of NCs [17], and the carrier charging time in NCs [14,15]. Recent studies give the variation of L_D as a function of electron – beam (e-beam) energy in the presence of uncapped Ge NCs on Si/SiO_2 structures [17]. It appears that the mean diameter of uncapped NCs affects the value of L_D and its behavior as a function of the e-beam energy, while the NCs density does not substantially affect L_D. Other parameters can also affect the minority carrier diffusion length, namely the distance separating each NC from the nano-contact collecting the current. For this, a Monte-Carlo simulation algorithm was used to study nano-EBIC in an intrinsic silicon sample which contains at its surface a linear arrangement of uncapped NCs. It has shown that an increase of the distance between each NC and the nano-contact reduces the effect of the charge trapping by the NCs and enhances the collection efficiency [18]. A threshold separation distance, from which NCs have no more effect on the collection efficiency, has been found, and the resulting minority carrier diffusion length reached the value obtained in the absence of NCs.

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However, remind that the NCs were on the surface sample. The situation will not be the same if the NCs are embedded in the sample under test. Here the capture will be made in the three directions.

The aim of this work is to study the collection efficiency profile in the presence of an embedded NC beneath the nano-electrode in the perpendicular direction to the sample surface at a distance which is varied to highlight its effect on the collection efficiency. Another aim of this study is to characterize the charge trapping process establishing in the NC as a function of its depth position. A Monte-Carlo simulation algorithm is used to help us to better understand the competition between the collection process by the nano-electrode and the capture process by the NC which is considered as a recombination center. This competition is studied as a function of the distance in depth which separates the NC from the nano-electrode. The simulation program takes into account of some significant parameters, namely; the size of the depletion zone formed between the nano-electrode and the sample, the bulk diffusion length which is considered to be independent of the primary energy and not affected by the presence of the NC, the mean radius of the spherical NC, the distance between the nano-electrode and the NC, and the e-beam energy. We also take into account of the charge collection and capture probabilities in the bulk of the studied sample, and we also take into account of the collection probability at the surface.

2. Rapid description of the Monte-Carlo simulation

To explain the electron sample interactions, the Monte-Carlo simulation algorithm is widely used in the literature, as quoted in many papers [19–29]. Our study is inspired from these previous works; we make some changes and add some calculation to take into account of the presence of NCs, the size and the shape of the nano-electrode, the probability of a created charge to be collected, captured by the NC, or recombined in the sample. Competition between probabilities of carrier collection by the nano-electrode and carrier capture by the NC is underlined. For clarity of the description, the geometry is given in Fig. 1. The half-circle represents the hemispherical shape of the depletion zone of radius r. A line of the sample is scanned along the y-axis passing through the nano-electrode; the e-beam irradiation is made in a perpendicular configuration. Two energy values are used; 1 keV and 5 keV. The NC has a radius r_n and it is situated at the depth z_n from the nano-electrode. The sample is irradiated in succession by 200 electrons one after another.

We first define the incident electron trajectory by the scattering angle (θ) and the azimuthal scattering angle (φ) as shown in Fig. 2. We also define the step between successive collisions. Since elastic collisions dominate, the primary electron energy is supposed continuously lost (see the *appendix*). The energy lost between two successive collisions is used to create n_{e-h} electron-hole pairs, given by:

$$n_{e-h} = \frac{\Delta E}{E_{e-h}} \tag{1}$$

where E_{e-h} is the electron-hole formation energy and ΔE is the energy lost between two successive collisions. Experimental measurements in different semiconductors give $E_{e-h} \approx 3 \times E_g$ [30], where E_g is the gap energy of the considered semiconductor. For silicon $E_{e-h} \approx 3.6$ eV.

We now describe how to follow each created charge. The position of created charges is assumed to be in the middle of the distance separating two successive diffusions. The random diffusion of the created charge is controlled by two angles α and β as shown in Fig. 2. α defines the orientation angle of the created charge trajectory and β is varied from 0 to 2π to take into account of all directions. These angles are given by:

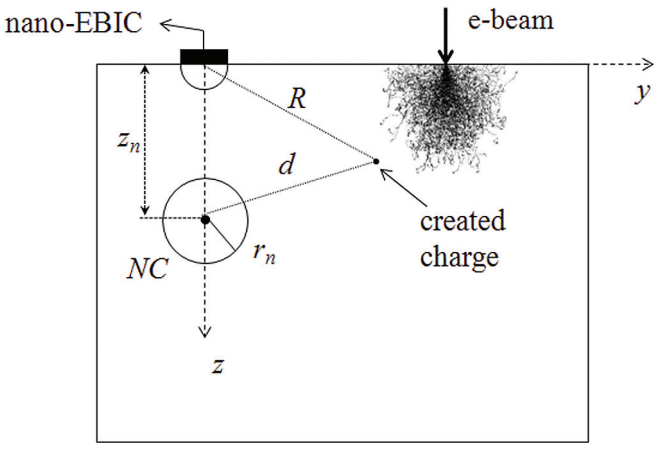

Fig. 1. A cross-sectional view of the schematic representation of the nano-EBIC procedure in the presence of an embedded NC just beneath the nano-contact at a distance z_n.