On the Effect of Local Electronic Stopping on Ion Implantation Profiles in Non-Crystalline Targets

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1 Introduction

The standard model for simulation of ion implantation into amorphous materials based on the LSS concept of ion penetration [1] remained a reliable work horse for the simulation of ion implantation for a long time, but recent accurate experimental measurements of the implantation profiles in non-crystalline materials (photoresist, amorphous carbon, pre-amorphized silicon) indicated systematic deviations of the measured profiles from the predictions of that standard model. The experimentally measured implantation profiles are usually broader than predictions of simulations based on the amorphous material model, and the relative profile broadening is especially significant for heavy ions at elevated implantation energies. Several physical effects may come in question to explain the broadening of the implantation profiles: experimental uncertainty during the profile analysis, radiation enhanced diffusion during ion implantation, deficiency of the physical model for ion-atomic interaction. The high accuracy of the measurements and the fact that the observed profile broadening is independent of the chemical nature of the target atoms and ions speaks in favour of the last assumption about the physical background of these deviations between the model and experiment.

2 Models of electronic stopping in non-crystalline materials

The standard model for simulation of ion implantation in amorphous material assumes that nuclear collisions and electronic stopping are independent, with electronic stopping being a function of ion energy and being position independent. The range straggling of the implanted ions in this model is mainly determined by nuclear collisions, the electronic stopping acts merely as a continuous friction force. From such a model it follows that the relative projected range straggling $\Delta R_p/R_p$ remains unchanged when electronic stopping is adjusted to reproduce the mean projected range R_p in a simulation. Moreover, the enlarged values of $\Delta R_p/R_p$ observed experimentally could not be reproduced in the simulation when different but realistic models for the nuclear scattering were tested. The position dependent local electronic energy loss is known to play an important role in channeling phenomena increasing the range of channeled ions. A similar increase of the ion ranges can also take place in amorphous materials if one considers that the electronic stopping in an amorphous material is strongly impact parameter dependent and therefore is strongly correlated with nuclear energy loss. In fact, the average electronic stopping of ions which have a maximum possible range, i. e. which predominantly participate in distant collisions, is then expected to be lower than for the mean stopping of the ions and such ions therefore have a larger projected range than predicted by standard models leading to an overall increase of the profile width.

An attempt to quantitatively describe the effect of the widening of ion implantation profiles in non-crystalline materials used in semiconductor technology due to position dependent local electronic energy loss was done in this work. To describe channeling phenomena, an exponential dependence of the electronic stopping on the minimum approach distance between ion and the target atom was suggested by Oen and Robinson [2]. The energy loss in a single collision, $T_e(E, p)$, as a function of the ion kinetic energy, E, and the impact parameter, p, is described as:

$$T_{e}(E, p) = A S_{e} \exp\left[-B r_{0}(E, p)/a\right],$$
(1)

where A is the normalisation coefficient to ensure the proper value of the total electronic stopping cross section S_e which is the measure of the average electronic stopping, B is the model coefficient which determines how sharply the energy loss T_e decreases if the impact parameter p increases, a is the inter-atomic screening length, and r_0 is the distance of closest approach in a collision at ion energy E and impact parameter p. A value of 0.3 was suggested originally by Oen and Robinson for the constant B to describe the channeling phenomena. Later, Xia et al. [3] applied the impact parameter dependent energy loss of Eq. (1) to describe ion implantation into crystalline silicon in non-channeled directions and for ion implantation into amorphous carbon. Larger values of B equal to 0.45 and 0.76 were found to describe ion implantation into action and phosphorus, respectively, into silicon and B=0.4 was found for argon implantation into carbon.

3 Simulation results, comparison to experiment

To simulate the implantation profiles, a modified Monte-Carlo code of the TRIM program [4] was used in this work. The standard model for amorphous materials included a position independent electronic stopping according to Ziegler-Biersack-Littmark (ZBL) tabulation [4], and the maximum impact parameter in the simulation was energy dependent so that only a part of all possible impact parameters were considered at elevated implantation energies. The model suggested in this work used an impact parameter dependent local electronic stopping according to Eq. (1) with B=1, the average electronic energy loss was equal to the ZBL tabulation or in some cases corrected with a constant energy independent scaling factor to reproduce the average projected range in the simulation, and the maximum impact parameter was energy independent and equal to the half distance between next neighbours in the amorphized target material. The choice of the constant maximum impact parameter in

the present work prevents the unwanted limitation to small impact parameters at higher energies in TRIM program and distinguish our model from the model of Xia et al. [3].

Figures 1 to 4 show some of the results of simulations using the standard and new simulation models in comparison to the experimental results of Glawischnig and Parks [5] obtained for ion implantation of arsenic and phosphorus ions into photoresist. The best reproduction of the experimentally observed profiles in the simulation has been achieved with the model suggested in this work using the impact parameter dependent model for electronic stopping with a screening length equal to the screening length of inter-atomic interaction, i.e. B=1 in Equation (1).



Fig. 1. Implantation profile of arsenic in photoresist



Fig. 2. Implantation profile of phosphorus in photoresist



Fig. 3. Mean projected range of arsenic ions in photoresist as a function of implantation energy



Fig. 4. Mean projected range straggling of arsenic ions in photoresist as a function of implantation energy

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