Initial Conditions for Transient Enhanced Diffusion: Beyond the Plus-Factor Approach

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Abstract

A new model is proposed for interstitial and vacancy profiles due to ion implantation. When used in TED simulations, more accurate results are obtained than with the "plus-factor" model. The user is not required to run Monte Carlo simulations nor to explicitly take spatial correlations between interstitials and vacancies into account. The model is formulated in terms of effective Frenkel pair numbers and vertical and lateral shift distances between interstitial and vacancy profiles. It is well suited for 1D/2D/3D process simulation.

1 Introduction

According to the "plus-factor model" the initial interstitial profile for transient enhanced diffusion (TED) simulations is assumed to be the as-implanted dopant profile multiplied with the "plus-factor". The plus-factor has been determined in [1] as to yield the same amount of diffusion in the bulk as simulations using the full point defect distributions. Values as large as 4 have been found for practical implant conditions (a value of unity corresponds to the "+1" model [2]). The origin of plus-factors different from unity are deviations between the interstitial (I) and vacancy (V) profiles, with net-excess interstitials (netI) deeper in the bulk and net-excess vacancies (netV) near the surface, and the out-diffusion of vacancies during Frenkel pair recombination.

While the plus-factor model is a major improvement over the "+1" model, it still has limitations: (i) The depth dependence of TED is not accurately described. When the plus-factor is calibrated in the bulk, errors up to 20% may occur at $x = R_p$ and even larger errors near the surface [3]. (ii) There is no information about the number of Frenkel pairs. Therefore, it cannot be used to simulate processes taking place during Frenkel pair recombination such as the competition between dopant-interstitial and interstitial-interstitial clustering [4]. (iii) While the plus-factor model can be applied to amorphizing implants, the plus-factors assume high values and depend on both the implant energy and the dose, as will be shown. This complicates finding an analytical expression for the plus-factor as a function of the implant parameters [3].

In order to overcome these problems, we propose alternative ways of constructing I and V profiles as initial conditions for TED simulations. They are more accurate than the plus-factor model but avoid the complexity of the original model [1, 5]. In the following we present models for non-amorphizing and amorphizing implants (Sections 2 and 3, respectively), and extend these models to two and three spatial dimensions (Section 4).

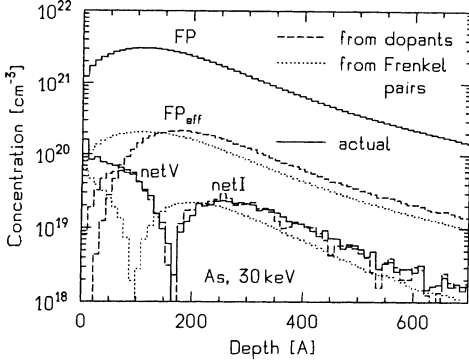

Fig. 1: Construction of effective point defect profiles after a non-amorphizing implant by scaling and shifting the dopant profile (dashed lines) and the Frenkel pair (FP) profile (dotted lines). netI=max(I-V,0), netV=max(V-I,0).

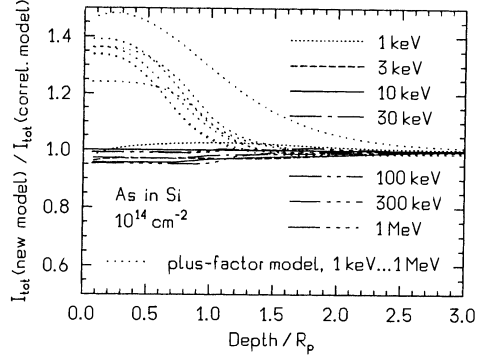

Fig. 2: Ratio of the time integrated interstitial supersaturations calculated with the proposed model and with the more sophisticated model of [1, 5]. For comparison the corresponding ratio is shown for the plus-factor approach by the wide-dotted lines.

2 Non-amorphizing implants

The first feature to be eliminated from the original model [1, 5] are the spatial correlations between I's and V's. We do this by scaling the I and V profiles such that the scaled profiles together with the standard recombination rate $4\pi r_0 D C_\mathrm{I} C_\mathrm{V}$ yield the same amount of TED as the actual profiles together with the more sophisticated recombination model [1, 5]. The scaling factor, which can be written as the ratio of the corresponding numbers of Frenkel pairs per ion, may be estimated as

$$n_\mathrm{FPeff}/n_\mathrm{FP} = \left(1 + 4\pi r_0 D \int_0^\infty w(t)\,\mathrm{d}t\right)^{-1} \tag{1}$$

using the theory developed in [1] and assuming that correlations disappear quickly from the distribution. r_0 denotes the capture radius, D the sum of the I and V diffusivities, and $w(t)$ a function defined in [1] that contains information about the spatial correlations. Alternatively, $n_\mathrm{FPeff}/n_\mathrm{FP}$ can be determined by comparing TED simulations with and without correlations. The two approaches agree reasonably well.

The second task is to construct the scaled vacancy profile $C_\mathrm{Veff}(x)$ from the scaled interstitial profile $C_\mathrm{Ieff}(x)$. This allows to use analytical expressions for $C_\mathrm{Ieff}(x)$ [6], to determine $C_\mathrm{Ieff}(x)$ from Monte Carlo simulations with poorer statistics, or to approximate $C_\mathrm{Ieff}(x)$ by the scaled dopant profile $C_\mathrm{A}(x)$. Following [7], we have tried to construct $C_\mathrm{Veff}(x)$ by shifting $C_\mathrm{Ieff}(x)$ towards the surface by some distance Δx. Fig. 1 shows that the resulting netI and netV profiles (dotted lines) do not agree well with the corresponding profiles determined from the actual I and V distributions (solid lines). Much better results are obtained by using the scaled dopant profile (dashed lines):

$$C_\mathrm{Ieff}(x) = n_\mathrm{FPeff} C_\mathrm{A}(x), \qquad C_\mathrm{Veff}(x) = C_\mathrm{Ieff}(x + \Delta x). \tag{2}$$

With properly chosen parameters n_FPeff and Δx the depth dependence of TED is much better described than by the plus-factor model. In the example shown in Fig. 2 the maximum error is reduced from 50% to 5%.

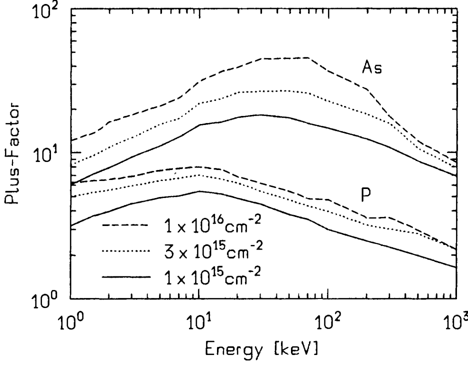

Fig. 3: Plus-factor as a function of energy for P and As ions at three amorphizing implantation doses. Note the dose dependence.

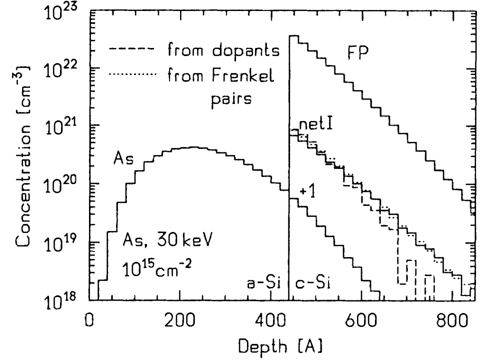

Fig. 4: Construction of net-excess interstitial (netI) profiles after an amorphizing implant by shifting the Frenkel pair (FP) profile (dotted lines) and the scaled dopant profile (dashed lines).

3 Amorphizing implants

For amorphizing implants it is assumed that recrystallization sweeps away all point defects within the amorphized zone. Because of the high concentrations in the remaining profile, recombination is fast and all that matters is the netI distribution [8]. Therefore, I–V correlations are not an issue. Plus-factors can be determined in the same way as in the case of non-amorphizing implants. Fig. 3 shows that large values are obtained, particularly for the heavy ion species As. Moreover, the plus-factor significantly depends on the dose. This is explained by the flatter tails of the point defect distributions compared to the dopant profile. Thus, when the amorphous zone increases, larger scaling factors are needed to obtain approximate netI distributions from the dopant profiles.

For the same reason it is better to use the actual interstitial profile than the scaled dopant profile in a model similar to that proposed in Section 2. An example illustrating this is given in Fig. 4. The netI profile is obtained by

$$C_{\mathrm{netI}}(x) = C_{\mathrm{I}}(x) - C_{\mathrm{V}}(x) \approx C_{\mathrm{I}}(x) - C_{\mathrm{I}}(x + \Delta x) \approx -\frac{\partial C_{\mathrm{I}}}{\partial x}\Delta x. \tag{3}$$

The interstitial profiles can be approximated by the analytical functions published previously [4]. The shift distance Δx is independent of the implant dose in contrast to the plus-factor in the plus-factor model (Fig. 3).

4 Two- and three-dimensional model

Fig. 5 shows the two-dimensional distributions of netI's and netV's after implantation by a mask edge, calculated by shifting the vertical distribution function as described above and using the same lateral distribution function for I's and V's. With this approach netV's appear near the surface, which clearly disagrees with the actual 2-D Monte Carlo results (solid lines in Fig. 6). The deficiency can be repaired by shifting the lateral I distribution $f_{\mathrm{I}}^{\mathrm{lat}}(y)$ away from the center by a distance Δy. The dose added

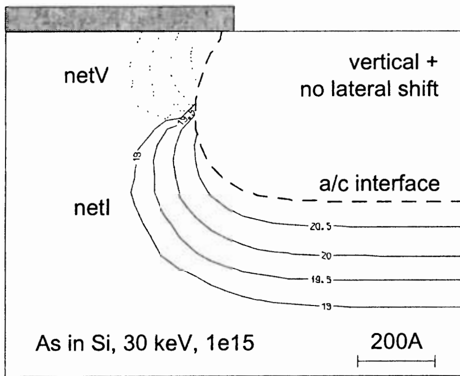

Fig. 5: 2-D net-excess interstitial (netI) and vacancy (netV) distribution calculated from shifted vertical and identical lateral I and V distribution functions. The presence of netV's near the surface is in disagreement with the full Monte Carlo simulations (see Fig. 6).

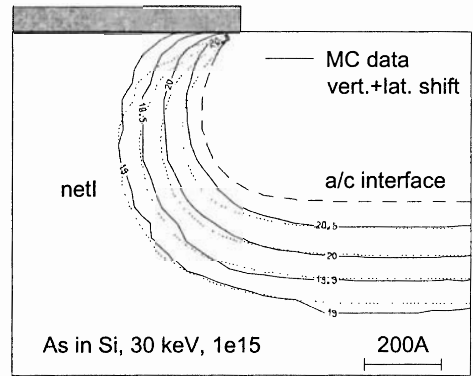

Fig. 6: 2-D net-excess interstitial (netI) and vacancy (netV) distributions as obtained from Monte Carlo simulations (solid lines) and by shifting the vertical and the lateral distribution function (dotted lines). In both models there are no netV's near the surface.

in the center can be compensated for by subtracting a Gaussian function with a standard deviation σ, which has to obey $\Delta y \ll \sigma \ll \sigma_{\mathrm{lat}}$ with σ_{lat} the standard deviation of the lateral V distribution:

$$f_{\mathrm{I}}^{\mathrm{lat}}(y) = f_{\mathrm{V}}^{\mathrm{lat}}(\max(|y| - \Delta y, 0)) - \frac{2\Delta y f_{\mathrm{V}}^{\mathrm{lat}}(0)}{\sqrt{2\pi}\sigma} \exp\left(-\frac{y^2}{2\sigma^2}\right). \qquad (4)$$

This model has Δy and σ as parameters where the value of σ usually is uncritical. Similarly, in 3-D such a shift can be performed in radial direction.

Thus, we have proposed a fairly simple and complete model of initial conditions for TED which can be used for 1D/2D/3D process simulation.

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