

Calculation of Ion Implantation Profiles for Two-Dimensional Process Modeling

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ABSTRACT

Advanced integrated circuit processing requires detailed modeling of each stage of the fabrication, to provide input for two-dimensional device models. This paper summarizes the various methods that are available for calculating ion implantation profiles in two dimensions, comparing the generality and expense of each approach. Some problems remain in modeling channeling and in verifying the results directly. Examples illustrate the range of problems that can be tackled successfully and the information that can be obtained.

1. Introduction

The continual progress in integrated circuit device processing requires the continual evaluation and improvement of process and device modeling capabilities if they are to be practically useful. Modeling inaccuracies, which in the past were hidden by long thermal treatments or the smoothness of potential gradients, now cause significant differences between theory and experiment. The latest device modeling programs^[1] use sophisticated numerical methods to solve detailed physical models for device behavior, taking as a starting point the physical structure and doping distributions generated by two-dimensional process models. This provides the motivation for improving process models, particularly where detailed knowledge of the doping concentrations is critical to device behavior. Ion implantation is the primary method for introducing dopant into silicon, so we require detailed understanding of implantation profiles

in two dimensions, for example, at the edges of the gate in a MOS transistor where current flow critically effects device performance.

Many techniques have been applied to the modeling of ion implantation, each with its own trade-offs of simplicity, flexibility, accuracy and cost. There is also a hierarchy of difficulty in the problems presented, depending on the planarity and composition of the structure to be implanted. This paper will compare the methods that are available, illustrating the problems that have been solved and the limitations that remain.

2. Calculation Methods

Any implantation can be viewed as the sum of implantations at each point across the surface of the wafer. The difference in complexity of the various structures that are implanted comes from the number and type of different point-response functions (PR) that must be calculated. Fig. 1 illustrates the hierarchy of targets that are possible. The simplest cases involve a single PR which is superposed over unmasked areas of the target. All the methods are capable of calculating a single PR for a bare silicon wafer. If the target is planar multilayered, the same principle of superposition can be used but the simpler methods require approximating the target layers by equivalent silicon thicknesses. More sophisticated methods are required when the surface or interfaces are highly non-planar, or for calculation of recoil effects. Accurate treatment of mask edges usually falls into the "highly non-planar" category because the edges are steep but not vertical.

2.1 Moments methods

The first calculation method applied to ion ranges was by Lindhard, Scharff and Schiøtt^[2] (LSS). This method considers the probability for an ion to travel a certain distance into the target. An integrodifferential equation is formed for this probability, using a differential scattering cross-section to describe the interaction between ion and target atom. The target is assumed to be homogeneous and isotropic so that the spatial variables can be eliminated by taking moments. The resulting equations can be

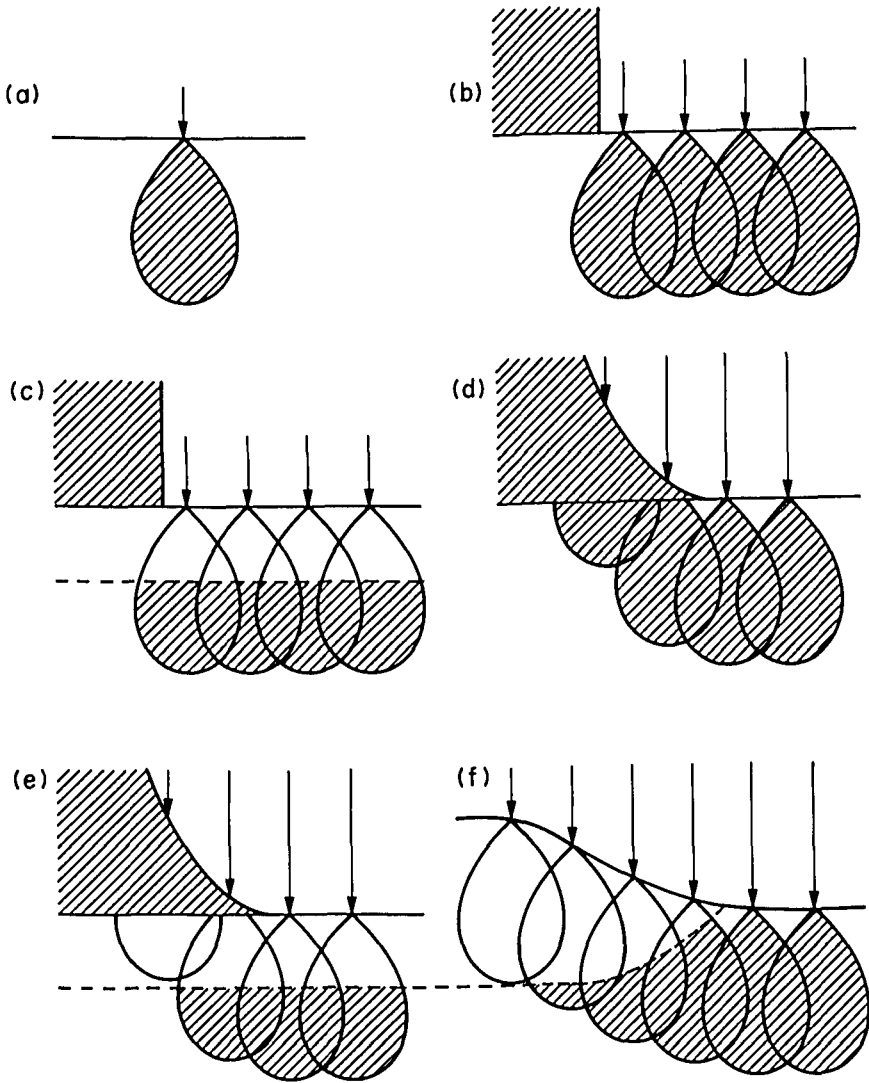


Figure 1. Examples of point-response functions (PRs) for various targets. a: Single-layer target. b: Vertical mask edge. c: Vertical mask and planar-layered target. d: Tilted mask edge. e: Tilted mask and planar-layered target. f: Non-planar layered target.

numerically solved to yield the first few moments of the ion distribution. The initial work considered the one-dimensional case, but this was later extended to two dimensions^[3], to arbitrarily shaped mask edges^[4] and to multilayer substrates^[5]. By considering intermediate energy distributions, damage distributions can also be calculated^[6]. The approximations used begin to break down when the target is far from planar, because of ions ejected from the surface, and where the layers are of dissimilar materials, because of the differences in scattering properties. However, this approach is easy to implement and takes little computation compared to other schemes, so it has been used in all the existing two-dimensional simulators.

2.2 Construction from projections

Full two-dimensional calculations are expensive to perform, so it is worthwhile to consider how much information can be obtained from Boltzmann or Monte Carlo methods with only one-dimensional effort. This is the idea behind construction of the two-dimensional PR from one-dimensional projections^[7]. In practice, it is sufficient to calculate the vertical and lateral one-dimensional projections of the profile. The PR is formed by taking the product of these two distributions. For the Boltzmann transport method, this requires two one-dimensional calculations; for Monte Carlo, the same number of ion tracks are considered as in a one-dimensional calculation. Fig. 2 compares such a construction with a direct, two-dimensional calculation for 20keV boron implantation into silicon, using a Monte Carlo method^[8], showing that the construction using only 10^4 ion tracks reproduces over the first two decades the full calculation using 10^6 ion tracks.

The limitations of the projection method are broadly the same as for moments methods because both superpose a single PR across the exposed region of the target. We can also obtain PRs for deposited energy and for displaced substrate atoms, so we can estimate stoichiometry disturbances in compound semiconductor targets, but we cannot calculate recoils across non-planar interfaces.

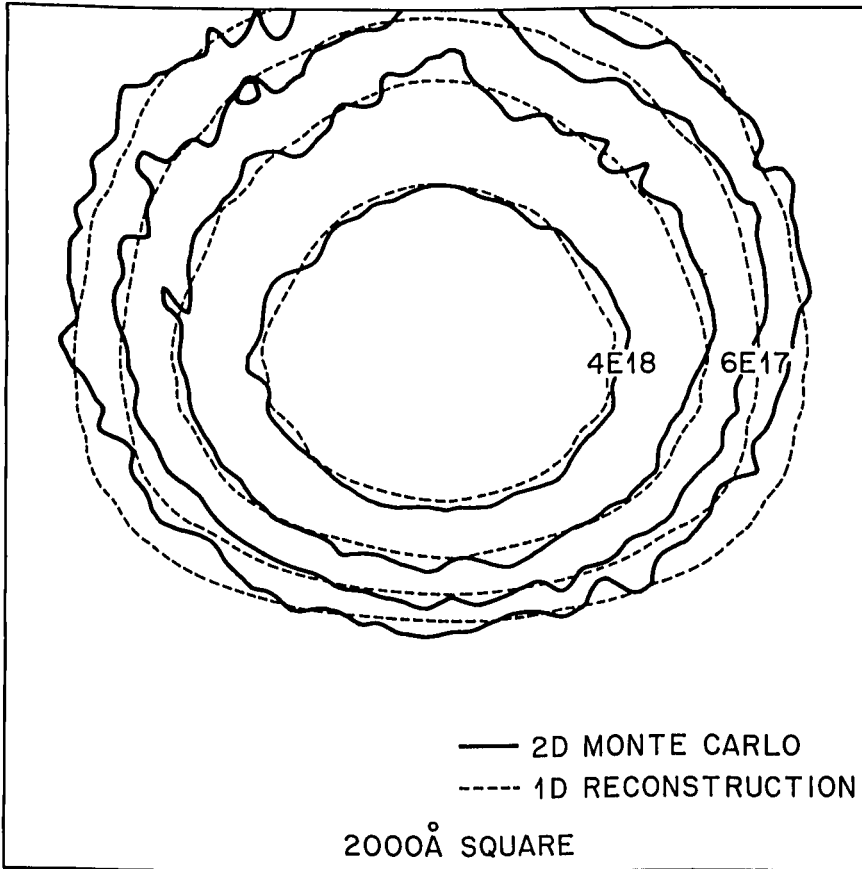


Figure 2. Comparison of a direct two-dimensional Monte Carlo calculation (10^6 ions) with a reconstruction from projections (10^4 ions) for 20keV boron implanted into silicon at a dose 10^{16} cm^{-2} .

2.3 Monte Carlo method

In a Monte Carlo calculation^{[8][9][10]}, the motion of individual ions is followed one-by-one as they are scattered by target atoms until they finally come to rest. The number of ions we need to follow depends on the accuracy desired -- in one dimension, 10^4 ions is usually enough. In two dimensions, there are two levels of calculation possible. The simplest is to calculate the PR directly by forcing all the ions to start at a single point on the target surface. The PR can then be superposed across the target as with previous methods. This requires at least 10^6 ion tracks for reasonable results, but now can

consider accurately planar interfaces. For a general target structure, ions must be started at all points across the target surface. There is no restriction in principle to the shape or composition of the target layers, but we must now follow 10^8 ions per unit of target width, where a unit is roughly the width of the corresponding PR. This rapidly becomes unmanageably large and offers no practical prospect for three-dimensional work.

2.4 Boltzmann transport method

In a Boltzmann transport calculation^{[11][12][14]}, all of the ions are considered together by following their statistical momentum distribution. Scattering by target atoms causes this distribution to change as the ions move through the target until they finally come to rest. As with a Monte Carlo calculation, we can choose between calculating a single PR and superposing, or calculating across the full width of the target directly. Calculation time scales linearly with the width of the simulation region just as with a Monte Carlo method, but typically a factor of 10 faster. There is no restriction in principle to the shape or composition of the target layers, and we can also calculate damage, recoil and stoichiometry effects just as in one dimension. An advantage of the Boltzmann method for recoil ion effects is that the calculation time is proportional to the number of ion types rather than the total number of ions. Since each incident ion generates many recoils, this is a further significant saving over Monte Carlo methods.

2.5 Other issues

A problem that pervades all two-dimensional process modeling is the difficulty of direct measurement of two-dimensional concentration profiles. Some techniques can resolve junctions in two-dimensions^[15], but this is far from the power in one dimension of SIMS or RBS analysis. For ion implantation, some lateral information can be inferred from one-dimensional analysis of tilted-beam implants^[16], which combines together components of the vertical and lateral profiles. The biggest obstacle to accurate profile calculation is channeling. Although some progress has been made in direct calculation^[17], most attempts have involved empirical fits to

experimental data^[18]. Since this information is not available in two dimensions, there is as yet no practical way to include channeling effects under a mask edge.

A further consequence of the refinements in integrated circuit device processing is that lateral diffusion distances have been significantly reduced. It is therefore becoming important to consider the asymmetry introduced by the standard 7° tilt used to reduce channeling effects. For example, there can be a variation in threshold voltage across a wafer due to different lateral penetrations of the implanted ions, which depends on the position and orientation of the transistor with respect to the beam tilt axis^[19]. All the calculation schemes described can be modified to include the effects of tilting the implantation beam, but a full-solution approach must be used if the details of scattering by sloping mask edges is to be considered.

3. Example calculations

A few example calculations will now be presented to illustrate the various methods that have been discussed. The simplest case involves implantation at a vertical mask edge, which can be solved using any of the above methods to generate a single PR then superposing across the exposed area of the substrate. Fig. 3 shows a calculation made with a moments method for a 50keV arsenic implanted into silicon. The PR is composed of a vertical Pearson distribution ($R_p = 370\text{\AA}$, $\sigma = 134\text{\AA}$, $s = 0.604$, $k = 3.50$) and a lateral gaussian distribution ($\sigma = 144\text{\AA}$). The same result would be produced by each method, to within its intrinsic accuracy, because the target is so simple. This calculation takes much less than 1s on a CRAY-XMP.

Fig. 4 shows the same implantation at a mask edge with a 63° slope angle, such as might be produced by chemical etching. For simplicity, the masking material is taken to be of the same stopping power as silicon. Calculated results are shown using the Boltzmann method in two ways: first, forming a single PR by considering implantation into a plain silicon target then superposing this across the entire surface of the masked target; second, a full calculation allowing arbitrary ion motion. The first calculation is representative

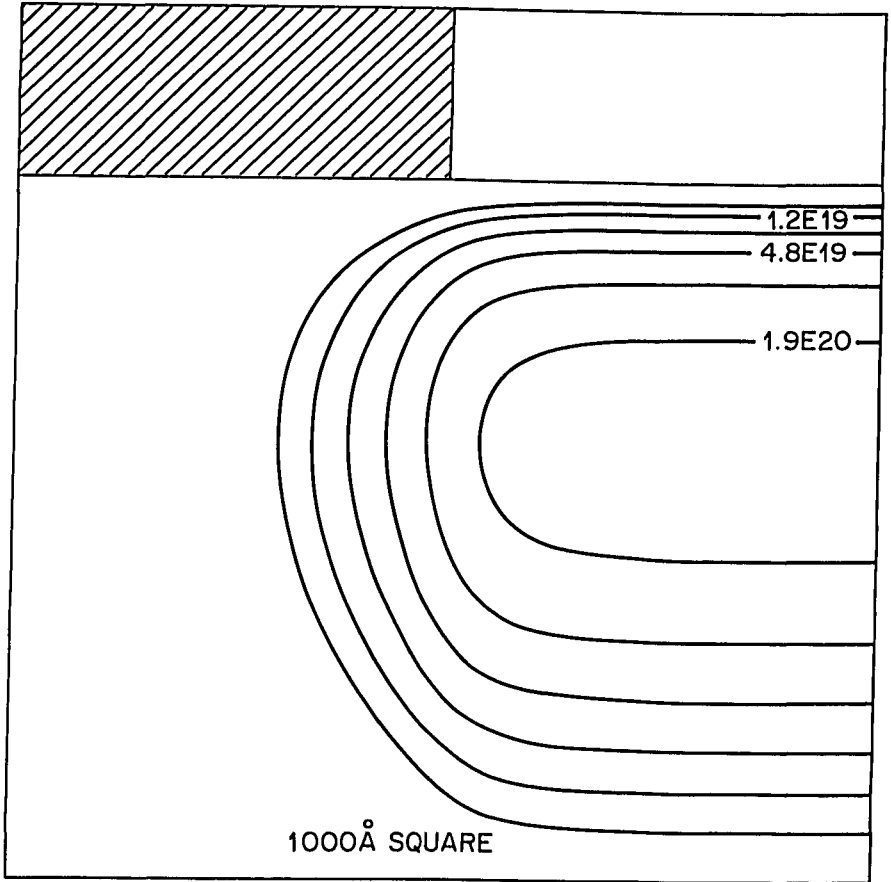


Figure 3. Implantation near a vertical mask edge, for 50keV Arsenic implanted into silicon at a dose 10^{16} cm^{-2} .

of all superposition methods, and the second of all direct calculations. The differences near the surface are due to ions that are scattered into free space from the sloping mask edge and then re-enter the silicon near the base of the mask. These ions have less energy than the directly implanted beam because of their initial scattering in the mask, so they form a shallow layer close to the mask edge. The bending of the contours in the superposition profile is a fortunate side-effect of the way the PRs are overlaid -- this effectively fills in the corner with silicon which scatters the ions, but any which stop are later removed because they are outside the true silicon boundary. Note the large differences between fig. 3 and fig. 4, due to the differences in the masks. These calculations took 76s and 150s respectively on a CRAY-1. If the single PR is formed from one-dimensional projections, it takes only 4s on a CRAY-1.

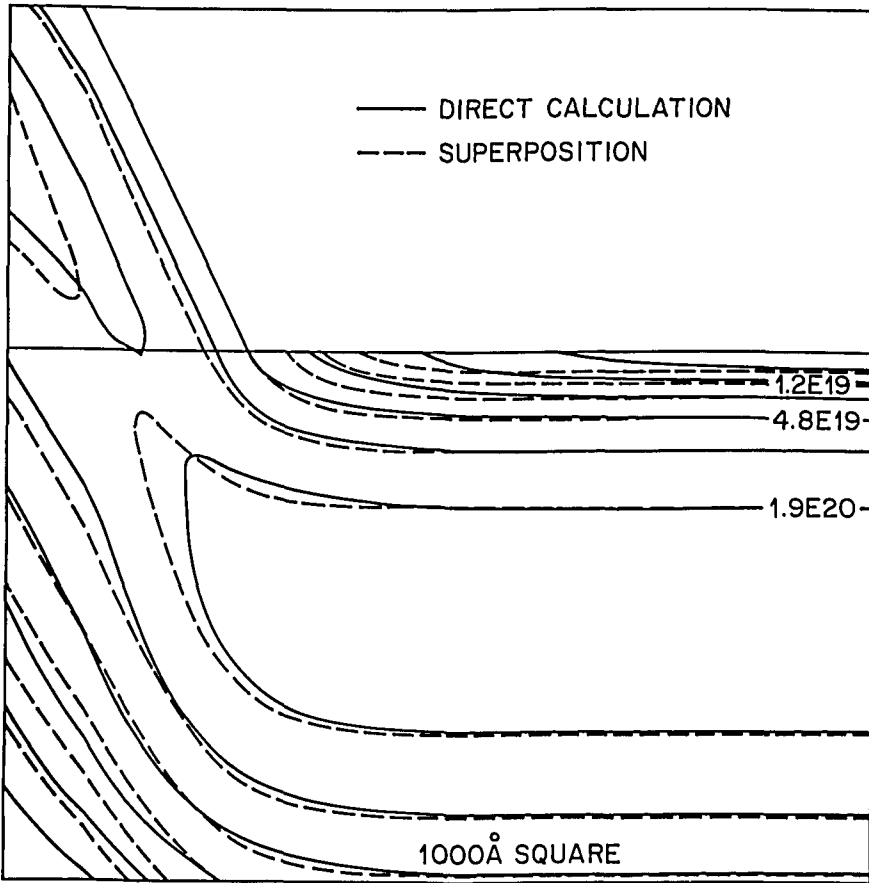


Figure 4. Implantation near a mask edge with 63° slope, for 50keV $^{16}_5\text{As}$ implanted into silicon at a dose 10^{16} cm^{-2} .

If recoils across non-planar interfaces are to be calculated, there is no choice but to use a direct calculation method. Fig. 5 shows such a calculation made with the Boltzmann method for oxygen recoils close to a LOCOS oxide edge. The concentration contours are for oxygen atoms only; the implanted arsenic profile is not shown. The recoiled oxygen profile forms an almost exponential tail away from the oxide region, as expected from one-dimensional calculations^[12]. Note also the thin line of oxygen atoms across the exposed surface, which were displaced from the side of the LOCOS oxide. At the interface, the recoil oxygen concentration (2E20) significantly exceeds the implanted boron concentration (6E19). This calculation was

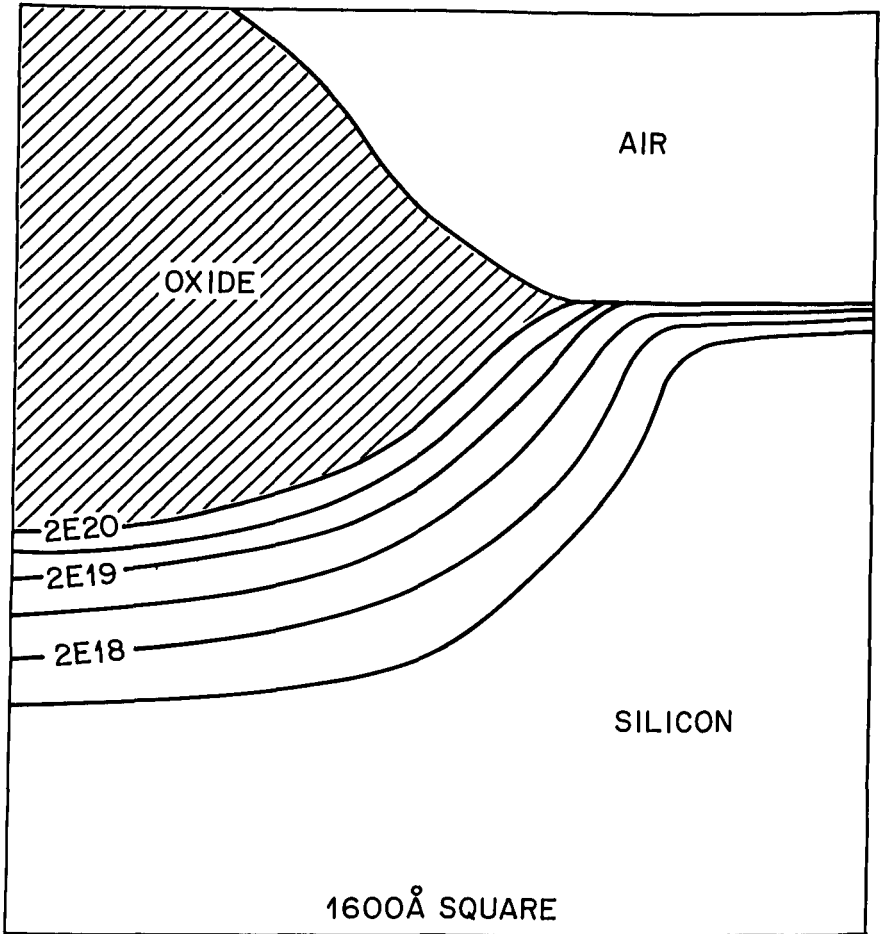


Figure 5. Oxygen recoils across a LOCOS oxide boundary caused by a 20keV boron implantation, dose 10^{15} cm^{-2} . The contours indicate the oxygen concentration only.

performed with the sides treated as reflecting boundaries, and took 400s on a CRAY-1.

Finally, fig. 6 shows a calculation made for implantation into a compound semiconductor, to consider the stoichiometry disturbance caused at the edge of a step. This must also be done with a direct method because of the non-planarity, and preferring Boltzmann over Monte Carlo because recoils are to be followed. The calculation shows material lost from both the top and side surfaces with net differences on the same order as the implanted ion concentration.

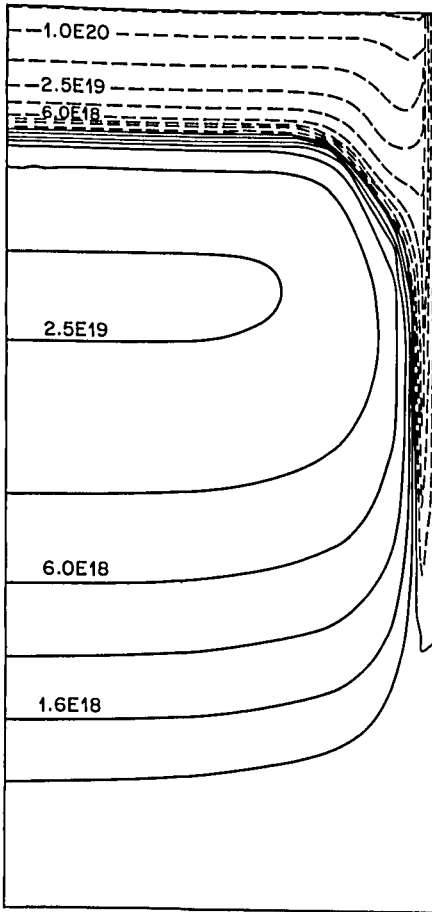


Figure 6. Net stoichiometry disturbance in GaAs near a vertical $^{16}_2$ step after a 50keV silicon implant, dose 10^{16} cm^{-2} .

4. Conclusions

Practical implantation modeling in two dimensions will require a hierarchy of methods. For most purposes, a simple superposition scheme is quite adequate. The more advanced methods need to be available for comparison at crucial areas of the device and to help diagnose problems such as can be caused by unwanted recoil effects. The calculation time of the more sophisticated models is not out of line with detailed modeling of other steps in the fabrication process, such as diffusion or oxidation.

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