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MODELLING DOPANT DIFFUSION IN POLYSILICON

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ABSTRACT

We present a model to describe the redistribution of dopant in and from an implanted planar polysilicon layer during a thermal anneal. The model incorporates the coupled processes of dopant segregation and grain growth in the polysilicon; the parallel diffusion of dopant along the grain boundaries and in the grain interior; and the diffusion of dopant into the underlying substrate. These processes are modelled fully in 2D with moving nodes employed to track the grain boundary motion. Validation of the model for the case of arsenic will also be presented.

INTRODUCTION

Polysilicon is widely used both as an interconnect and a diffusion source in VLSI technology. In current bipolar technology polysilicon is used as a such for both base and emitter. This requires an understanding of the diffusion process both within and from a polysilicon layer for both arsenic and boron. A model has been developed which is able to predict the dopant redistribution for both short and long anneals of a planar layer of as-implanted polysilicon on a single crystal substrate. The case for a short anneal in which only the dopant redistribution within the polysilicon layer is considered has been presented previously [1]. In this paper the extension of this model to fully couple the diffusion into the underlying single crystal substrate with that in the polysilicon will be described. (An approximation to this coupled model has been

presented previously [2]). The model is able to predict the full diffusion profile in the substrate; in particular it can predict any lateral non-uniformity on the scale of the polysilicon grain width which may arise due to the enhanced diffusion source where vertical grain boundaries meet the substrate interface. Validation of this model has been performed for the case of arsenic.

MODEL DESCRIPTION

The model incorporates the following physical processes which are believed to occur during thermal anneal of as-implanted polysilicon layers: the grain growth, and hence grain boundary motion, of the polysilicon from its as-deposited structure; the parallel processes of rapid dopant diffusion in the grain boundaries and the slow diffusion in the bulk grain interior; and the transport of dopant by grain boundary motion and segregation between grain boundary and grain interior sites. The polysilicon is treated as having a columnar grain structure (suitable for LPCVD poly) with an average lateral grain size which increases during thermal anneal to an equilibrium value approximately equal to the layer thickness. For the case of arsenic implanted polysilicon layers, the resulting amorphised implant region recrystallises to a larger grain size on heat treatment and so in this case the polysilicon is treated as having a two-level grain structure. The surface and the interface of the polysilicon with an assumed underlying single crystal are treated as extended lateral grain boundaries. To incorporate the above processes, which describe both lateral and vertical dopant transport, the model is necessarily 2D.

For a planar polysilicon layer it is sufficient to model the region of the polysilicon corresponding to a single equilibrium grain size, as all other regions are equivalent to this one. A schematic view of the dopant restribution mechanisms within such a region during thermal anneal is shown in figure 1. This shows a section through an assumed cylindrical grain which is expanding to occupy the full region shown. Dopant is transported rapidly along the vertical grain boundaries and is segregated within the expanding grain. It is necessary to follow the dopant concentration both within the grain interior, c (per unit volume), and at the grain boundary, c' (per unit area of grain boundary). The equation governing the concentration of dopant along the vertical grain boundaries is given by:

$$\frac{\partial}{\partial t}\left(\frac{c'}{L}\right) = \frac{\partial}{\partial y}\left(\frac{D'}{L}\frac{\partial c'}{\partial y}\right) + \frac{q}{L}\left(\overline{c} - Kc'\right) \qquad (1)$$

The first term represents diffusion along the grain boundary with diffusivity D'; the second term is a source term representing the combined effect of grain boundary motion (velocity q) and segregation (coefficient K) between the grain boundary

and the grain interior. The quantity $\overline{c}$ is the concentration of dopant in the region into which the grain expands (currently approximated as equal to the average of the interior grain concentration). Note that the equation is written in terms of c'/L, where L is the grain size; this scaling accounts for the enhancement in concentration as the grain boundary density reduces (enabling the total dose to be conserved).

The grain size is given as a function of time, t, as $L = \sqrt{L_0^2 + kt}$ [3] with L_0 and k fitted to measured grain sizes.

Along the lateral surface and interface grain boundaries the following diffusion equation is satisfied. An additional term is operative at the intersection with the vertical grain boundary to account for the dopant flux from the exterior as this point moves outwards (currently we assume that the exterior grain boundary concentration is the average of the interior):

$$\frac{\partial c'}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(D' r \frac{\partial c'}{\partial r}\right) + \delta(r-\tfrac{1}{2}L(t))\, q\, (\overline{c}'-c'(r)) \qquad (2)$$

Within the grain interior and the substrate the non-linear diffusion equation is satisfied:

$$\frac{\partial c}{\partial t} = \nabla(D(C_A)\ \nabla C_A) \qquad (3)$$

where D(c) is the concentration dependent diffusivity. The active concentration, c_A , is determined using an exponential relaxation to clustering equilibrium using the rate coefficients of [4]. Equation (3) is solved subject to the boundary condition that the grain edge is in segregation equilibrium with the grain boundary for both vertical and horizontal (interface) boundaries:

$$c = Kc' \qquad (4)$$

NUMERICAL PROCEDURE

In order to solve the above coupled set of equations (1)-(4) a finite difference representation is obtained on a 2D rectangular grid. In order to track the moving vertical grain boundary an adaptive grid is employed so that the boundary always coincides with a set of nodes. The edge region of the grid is shown in figure 2. The interior nodes are at a fixed spacing of Δ_0; the last two lateral nodes are equispaced but with a spacing varying between a minimum of $0.5\Delta_0$ and maximum of Δ_0 as the grain boundary moves a distance Δ_0. When a new lateral node is overtaken the mesh is re-defined with the minimum spacing of $0.5\Delta_0$ at the edge, with concentrations interpolated onto the new nodes.

The equations are solved with explicit time stepping. At each time step the grain boundary diffusion (1) is solved together with the grain growth and adaptation of the mesh. The diffusion in the interior grain (3) is then solved over this same time step subject to the boundary condition (4). The time step is limited by the large value of the grain boundary diffusivity; this potentially leads to a computing penalty since it over-restricts the time step for the 2D problem of equation (3). In practice for reasonable size grids this is not too severe.

MODEL VALIDATION

The model has been validated for the case of arsenic, implanted uniformly into planar polysilicon layers. Predictions of the 1D profile are obtained by averaging laterally and have been compared with measured SIMS profiles. As an example the case of a 30min 950°C drive-in of arsenic from a 0.2μm poly layer to the single crystal substrate is shown in figure 3. The key model parameter in this case is the segregation step at the interface, which was found to agree well with quoted values [5]. The single crystal diffusion coefficient was taken from [6]. Polysilicon grain sizes as a function of time have been measured from transverse TEM of implanted and annealed polysilicon layers.

RESULTS

Results from the model in the form of contour plots through a section of the polysilicon layer and underlying substrate are presented in the following. For the case of a 0.1μm LPCVD poly layer deposited at 620°C the initial average grain size has been measured as 100Å. When implanted with 30 keV 5E15 As^+/cm^2 the upper 600Å of the poly layer is amorphised, regrowing to a grain size of 300Å on heat treatment. The predicted arsenic distributions after 1ms and after 50s at 900°C are shown in figure 4. The distribution at the start of the anneal shows the initial segregation to the grain boundaries of the 2-level grain. The distribution after 50s shows the 2-level grain with the full arsenic distribution modelled in the interior and the substrate. The exterior region to the expanding grain takes the average concentration of the interior. It can be seen that, in this case, the substrate concentration is laterally uniform; this is a consequence of the fast diffusion along the interface grain boundary which is able to remove any lateral inhomogeneity. The arsenic has diffused to a depth of 60Å into the substrate.

Potentially larger lateral inhomogeneities could occur in the substrate for either thicker poly layers and/or higher deposition temperatures. In both cases the initial grain size would be larger than the case presented above, and so greater diffusion can occur into the substrate before the interface grain boundary achieves a uniform concentration. As an example the case of a 0.4μm poly layer with initial grain size of 0.1μm implanted with 1 E16 40 keV As and annealed at 900°C for 200s is shown in figure 5. The diagram shows the lower part of the polysilicon layer and substrate. The concentration at the interface is $5x10^{18}cm^{-3}$; at a depth of 50Å into the substrate the concentration varies laterally between 1 and $2x10^{15}cm^{-3}$. Due to the very steep arsenic front, the vertical variation in the 10^{15} contour is very small, as can be seen from Figure 5.

As an example of the use of the model for other dopants the case of a 4E15 60 keV BF2 implant into 0.2μm of poly is shown in figure 6 after an anneal of 100s at 900°C. The ratio of grain boundary to grain interior diffusion coefficients is reduced relative to the case of arsenic (see ref [7]) and so we may expect greater lateral non-uniformity in the substrate. The segregation of boron to the grain boundaries is reduced relative to arsenic; a value was estimated from the data presented in [8] (giving an order of magnitude less segregation than arsenic). The surface concentration at the single crystal is $10^{20}cm^{-3}$ and there is very little lateral non-uniformity in the substrate (<20%). It appears that the dominant transport mechanism for dopant is via the grain boundary network, though this depends critically on the amount of segregation that occurs, and on the assumption that all the dopant in the grain boundaries is mobile. Further validation of these predictions for boron is required.

CONCLUSIONS

A model to predict the redistribution of as-implanted dopant during thermal anneal has been developed. The model includes effects due to the parallel diffusion in grain interior and grain boundary, grain growth and hence grain boundary motion, and the segregation of dopant between grain and grain boundary. By coupling the single crystal substrate to the polysilicon via an interface grain boundary the model is able to solve the 2D diffusion in the substrate, and thus able to predict any lateral non-uniformity on the scale of a grain width. At present the model is restricted to planar polysilicon layers.

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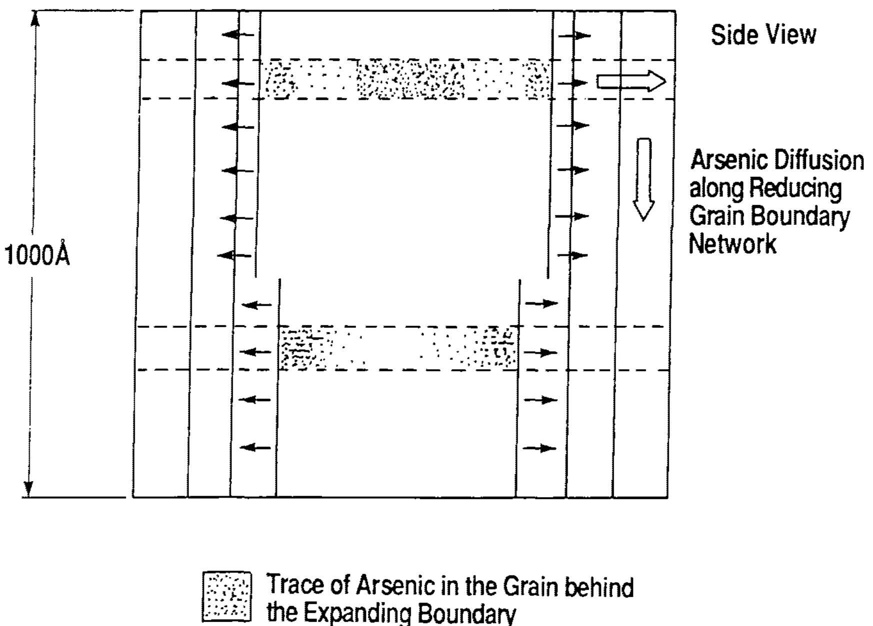

Figure 1: A schematic view of the dopant transport within a polysilicon layer as modelled. The expanding grain boundaries segregate dopant to the grain interior; rapid vertical diffusion occurs along the grain boundaries.

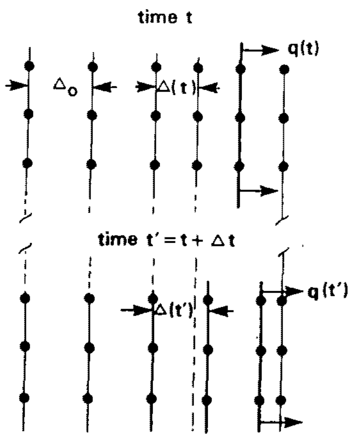

Figure 2 : The adaptive grid shown at two time steps. Only the nodes at the boundary and their neighbours move in order to track the moving grain boundary.

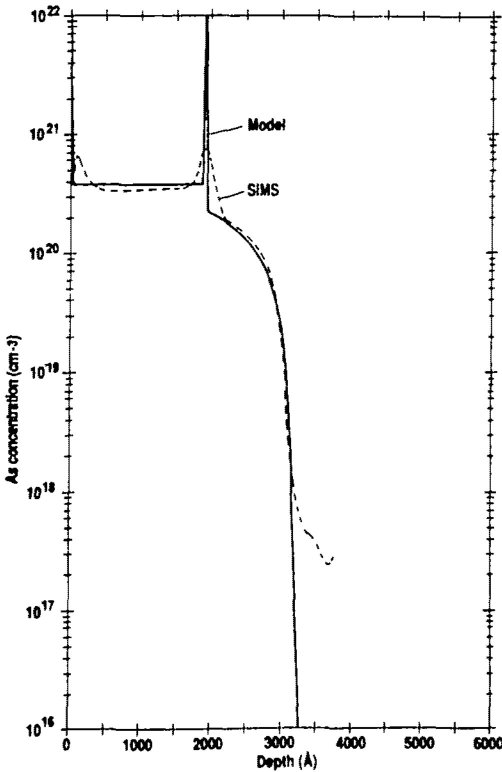

Figure 3: A comparison of the model prediction and the measured (SIMS) arsenic profiles for a $1x10^{16}As^{+}/cm^{2}$ 30keV implant into 1940Å polysilicon, annealed for 30 minutes at 950°C.

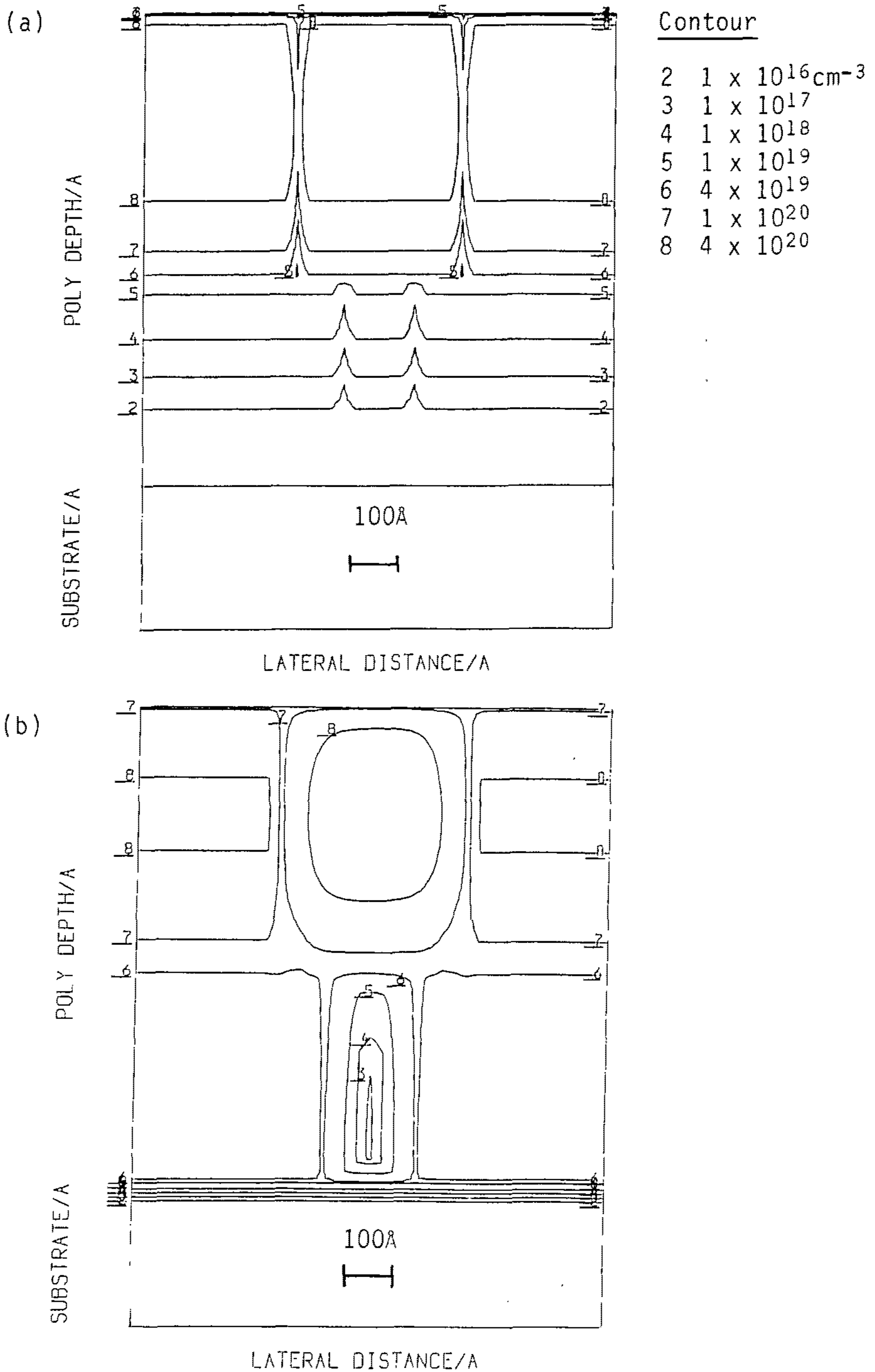

Figure 4: Model prediction for the arsenic distribution within a 0.1μ poly layer and substrate following a 5 x 10^{15} As^{+}/cm^2 30keV implant and 900°C anneal: (a) after ≈1ms; (b) after 50s.

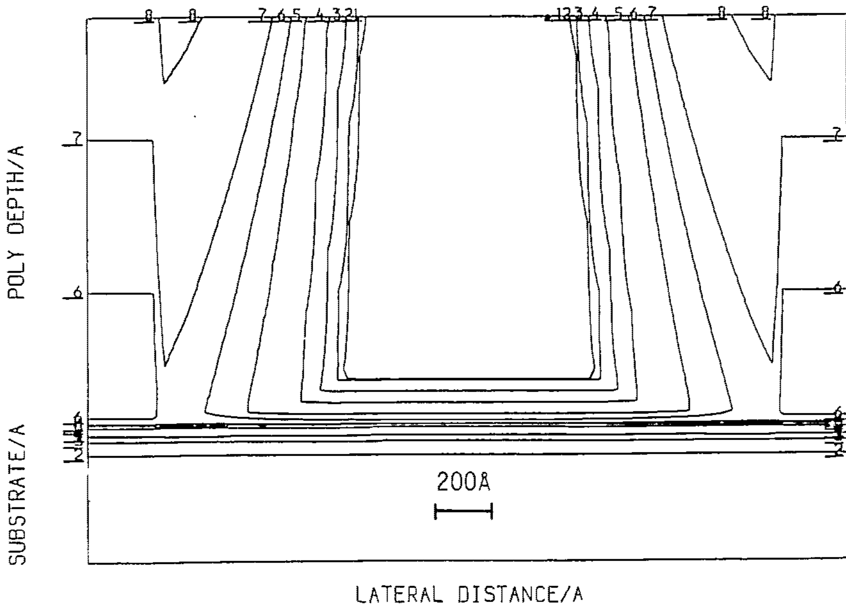

Figure 5: The Arsenic distribution in the lower 0.15μ of a 0.4μ poly layer and substrate following a $1x10^{16}As^{+}/cm^{2}$ 40keV implant and anneal at 900°C for 200s. Contours shown at 10^{12}, 10^{14}, 10^{16}, 10^{18}, $4x10^{18}$, 10^{19} and $4x10^{19}cm^{-3}$.

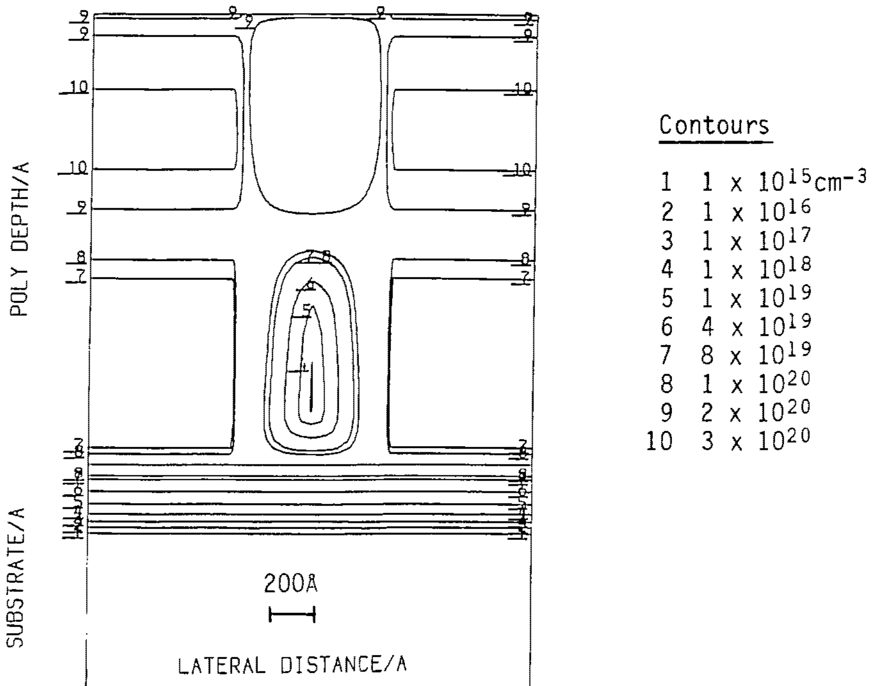

Figure 6: The boron distribution in a 0.2μ poly layer following a 60keV $4x10^{15}$ BF_2/cm^2 implant and 100s anneal at 900°C.