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Simulation of High-Dose Ion Implantation-Induced Transient Diffusion and of Electrical Activation of Boron in Crystalline Silicon

H. U. Jäger[‡†]

[‡]Research Center Rossendorf Inc.,
Institute for Ion Beam Physics and Materials Research
Postfach 510119, D-01314 Dresden, GERMANY
[†]Guest Scientist in the Fraunhofer-Institute of Microelectronic Circuits and Systems
Grenzstraße 28, D-01109 Dresden, GERMANY

Abstract

Coupled diffusion-reaction equations for boron and for point defects and rather simple initial conditions are used to model the implantation-induced transiently enhanced diffusion and the electrical activation of high-dose boron distributions during annealing.

1. Introduction

This investigation is dealing with the formation of shallow p^+-type regions in crystalline silicon by low-energy high-dose boron ion implantation and subsequent furnace annealing at low temperature (800°C). Figs. 1-3 show typical experimental data [1] as well as the respective results of our simulations. At 800°C, the normal boron diffusion is known to be negligible. In case of post-implantation annealing, however, both low-dose and high-dose boron profiles become modified in their tail regions up to a critical concentration c_{enh} of about 4×10^{18} cm^{-3}, which is far below the boron solid solubility limit $c_{sol}(800°C) = 3.2\times10^{19}$ cm^{-3}. This implantation-induced tail broadening relaxes within a time period of about 30 min. The non-diffusing boron in the profile peak region above c_{enh}, but below c_{sol}, is found to be partially electrically inactive. It becomes electrically active only after annealing periods of many hours.

The models applied to simulate the transient diffusion and electrical activation of boron at low temperatures range from pure phenomenological ones [1] to formulations [2, 3, 4, 5] which include explicitly reactions between dopant species and silicon point defects under nonequilibrium conditions. Our approach [5] which provided good results for low boron doses $D \lesssim 5\times10^{14}$ cm^{-2} has to be modified if the boron peak concentration in the sample significantly exceeds the solid solubility limit c_{sol}. The present conference contribution is aimed at a brief explanation of these model extensions. Some new simulation results for high boron doses are also presented (figs. 1-3), but a more complete discussion must be given elsewhere [6].

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*Guest scientist in the Fraunhofer-Institute of Microelectronic Circuits and Systems, IMS2, Grenzstr. 28, 01109 Dresden, Germany

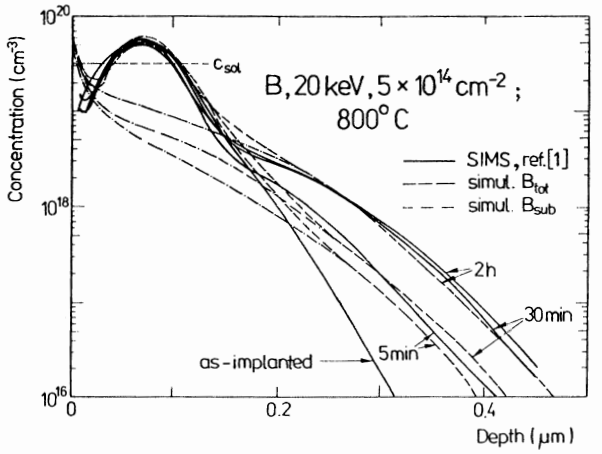

Figure 1: Time evolution of boron atomic (B_{tot}) and electrical (B_{sub}) profiles during 800°C furnace annealing after 20 keV 5×10^{14} cm^{-2} B ion implantation. The simulations are compared with profiles which have been measured by Solmi et al. [1] using secondary ion mass spectroscopy (SIMS).

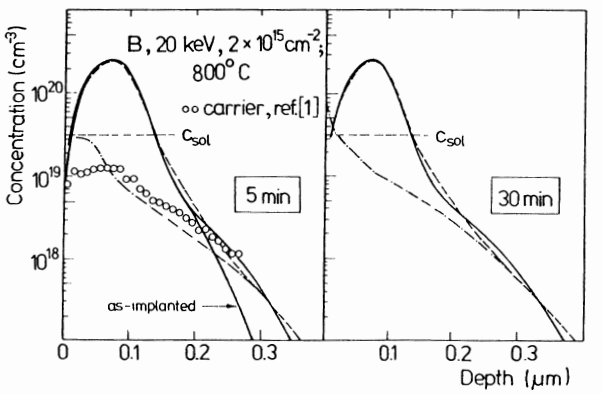

Figure 2: Model predictions and experimental profiles for a boron dose of 2×10^{15} cm^{-2}. The carrier profile has been measured [1] using anodic stripping followed by incremental sheet resistance and Hall effect measurements; for the other details, see fig. 1.

2. Basic model

The boron diffusion and activation have been modelled by solving a system of coupled diffusion-reaction equations. The species considered are boron atoms in solution on substitutional and interstitial sites (B^-_{sub}, B_{int}) as well as vacancies V^z and silicon self-interstitials I^z in various charge states z. The substitutional boron atoms and the point defects are assumed to form pairs ($B^-_{sub}I^z$), ($B^-_{sub}V^z$) in accordance with the mass action law. These pairs are the only diffusing vehicles (point defect impurity pair diffusion, [7]). The reactions, which are taken into account to simulate the change in activation during diffusion, are the kick-out reaction $B_{int} \Longleftrightarrow B_{sub} + I$, the Frank-Turnbull mechanism $B_{int} + V \Longleftrightarrow B_{sub}$, and the interstitial-vacancy annihilation and generation $I + V \Longleftrightarrow 0$.

The complicated details of defects evolution during ion implantation and during heating up to the annealing temperature are behind the scope of this study. Therefore a key problem of our approach is the finding of adequate initial conditions for the point defects and for the electrically active boron concentration B_{sub}. Let us postulate that a very early stage of annealing exists where diffusion is still unimportant,

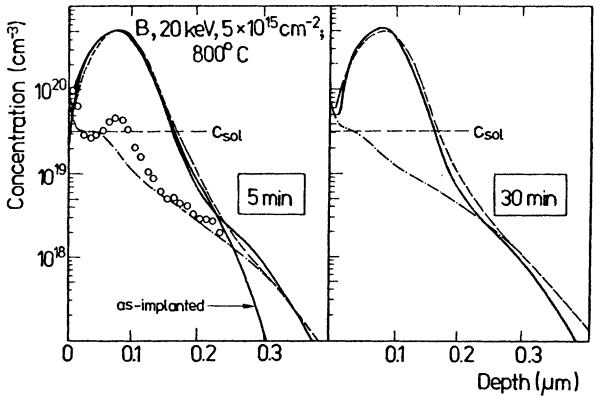

Figure 3: Model predictions and experimental profiles for a boron dose of $5\times10^{15}\,\mathrm{cm}^{-2}$. For details, see figs. 1 and 2.

but local equilibrium between the three reactions mentioned above is realized just at this moment. For a given total boron concentration, this local equilibrium is uniquely characterized by the concentration difference $Q = c_I - c_V - c_{B,sub}$, which represents the characteristic quantity of the given reactive species ensemble.

For low boron doses, an assumption of $Q = 0$ proves to be reasonable for all depth intervals in defining the initial conditions . A value $Q = 0$ can be thought to be originally realized by $c_I = c_V$, $c_{B,sub} = 0$ or by by $c_I = c_{B,sub}$, $c_V = 0$. Computing the local equilibrium for $Q = 0$ [5], one obtains initial conditions of the type $c_{B,sub} \approx c_I$, $c_V \ll c_I$.

3. High boron doses

For higher boron doses, of course clustered boron atoms B_{clus} must be taken into account. In our code, the boron concentrations exceeding c_{sol} are assumed to be completely clustered in the beginning

$B_{tot}=B_{sub}+B_{int}+B_{clus}$, with $B_{clus}=B_{tot}-c_{sol}$ for $B_{tot} > c_{sol}$;

precipitation models [1] have not yet been introduced.

The main problem of a straightforward point defect diffusion model seems to be the explanation of the experimental result that the boron profile broadening in the tail becomes nearly independent on the actual value of the high boron dose (compare, e.g., figs. 2 and 3). If our values [5] for the diffusion coefficients, the reaction rates and the point defect equilibrium concentrations c_I^*, c_V^* are not essentially changed, the initial conditions for implantation-induced diffusion in high-dose boron profiles can't be defined by $Q = 0$. The interstitial oversaturation affecting boron diffusion must be limited. In the present simulations we have used interstitial distributions whose peaks have been shifted in dependence on boron dose, so that the interstitial and boron profile tails will nearly coincide. A constant interstitial area density of 3.3×10^{14} cm^{-2} has been used. Furthermore, a complete activation of the solved boron atoms and equilibrium vacancy concentrations (c_V^*) have been assumed in the beginning. These details are illustrated by fig. 4a. The effect of the subsequent local equilibration is shown in fig. 4b. The model modifications explained so far are not yet sufficient to reproduce a dose-independent boron profile broadening. The outdiffusion of the interstitial oversaturations is retarded for increasing boron doses if increasing depths of the initial interstitial distributions are used. In order to compensate this effect,

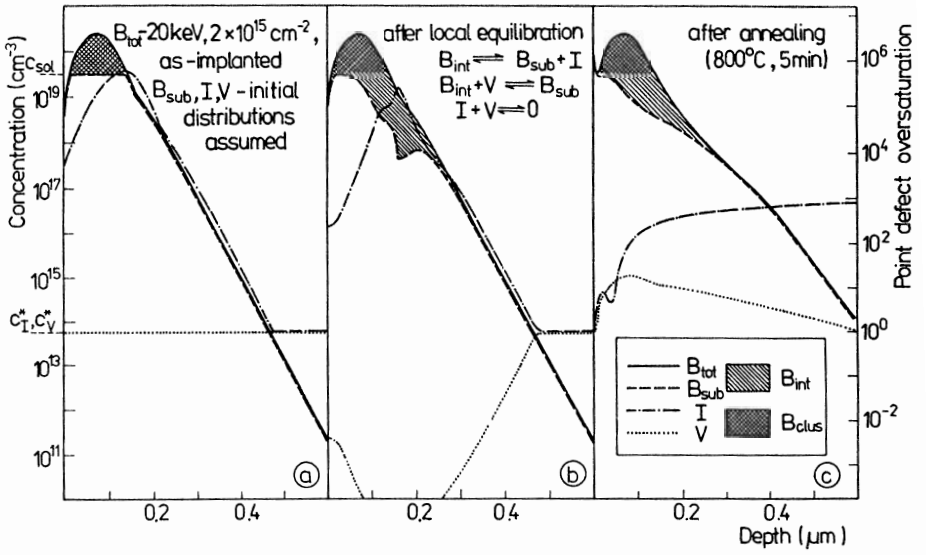

Figure 4: Illustration of the model components and of the predicted relations between boron profiles (left-hand scale) and point defect profiles (left- and right-hand scales) for an 800°C 5 min annealing after 20 keV 2×10^{15} cm^{-2} B ion implantation.

one can take into account that transitions of boron atoms from clusters into solution should affect directly the silicon point defect distributions. Such a correlation exists also in the dynamic clustering model of Cowern et al. [2]. We have assumed that the transition of one boron atom from a cluster onto an interstitial site (B_{int}) and the inverse process are accompanied by the annihilation or generation, respectively, of one silicon point defect. This process, which is described by the reactions $B_{clus} + I \Longleftrightarrow B_{int}$, $B_{clus} \Longleftrightarrow B_{int} + V$, seems to be necessary to obtain in the framework of our approach reasonable diffusion profiles for high boron doses (figs. 2, 3).

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