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Modelling the self-organization of boron clusters in silicon

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Abstract. The paper illustrates application the theory of self-organization to practical problems in the physics on nanostructures. Starting from the principles of the theory of self-organization, the formation of dissipative structures as found experimentally in annealed highly-boron-doped silicon samples is explained. A qualitative "reaction-diffusion" model is developed which reproduces the formation of spatially ordered boron clusters distribution in the form of equidistant maxima. Perspectives of more exact quantitative models describing the extraordinary evolution of boron dopant in silicon are discussed.

Introduction

This work gives an insight into understanding of the unusual behavior of boron dopant in silicon found experimentally beforehand [1–3]. In the experiment [1–3] the boron-doped crystalline silicon samples were additionally enriched in boron by ion implantation. The implantation led to an approximately 1000 nm-wide oversaturated region containing up to $4 \div 8 \cdot 10^{20}$ boron atoms per cm^3. The highly doped samples were annealed and the resulting depth distributions of the dopant were analyzed by SIMS. After annealing at 900–1075°C, complicated nonmonotonous boron distributions with several maxima and minima of the boron concentration were observed within the implanted oversaturated region. The distance between neighbouring maxima (peaks) close to 100 nm was found unchanged during the annealing and independent on the width of the implanted region. The latter, however, was crucial for the number of the peaks observed.

Thus, annealing of the boron-enriched silicon leads to a spontaneous spatial ordering of the dopant distribution. In this work a physical model is proposed to explain this unusual phenomenon.

1 Self-organization and formation of structures

In modern usage the spontaneous spatial ordering is known as self-organization and formation of dissipative structures [4–6]. From the theory of self-organization it follows that the transformation of homogeneous spatial component distributions into inhomogeneous ones can occur in open multicomponent systems of the Reaction-Diffusion type including interconversions of the system's components. The simplest mechanism leading to formation of spatially ordered structures such as a number of equidistant peaks can be conceived as a combination of positive and negative feedbacks (see e.g. [6]), with two principal elements being as-called short-range activation (self-maintaining of the peaks growth) and long-range inhibition (suppression of new peaks in a neighbourhood of one well developed).

In the present work we take the above fundamental results as a basis for our model of the self-organization process in hidhly doped silicon.

2 The model and its results

In refs. [1, 3] diffusion was suggested as the main mechanism of boron redistribution in the oversaturated samples, and the formation of the stable equidistant peaks was attributed to clusterization of the excess dopant.

In the present work, from the general principles of the theory of self-organization [4–6] it is shown that the spatial ordering of boron requires an active assistance of (at least) one further component — mobile crystalline defects. A straightforward one-dimensional model is put forward which explains spontaneous formation of the equidistant peaks in the boron depth distribution. The model includes diffusion of free boron dopant (f), precipitation of the excess boron into immobile clusters p ($f \to p$), and dissolution of the clusters ($p \to f$) with assistance of the third component — the hypotetic mobile defects d. The general form of the model is

$$\frac{\partial}{\partial t}C_f(x,t) = \frac{\partial}{\partial x}\left(D_f\frac{\partial}{\partial x}C_f(x,t)\right) - Q_1(C_i) + Q_2(C_i)$$

$$\frac{\partial}{\partial t}C_p(x,t) = Q_1(C_i) - Q_2(C_i)$$

$$\frac{\partial}{\partial t}C_d(x,t) = \frac{\partial}{\partial x}\left(D_d\frac{\partial}{\partial x}C_d(x,t)\right) - \alpha_1 Q_1(C_i) + \alpha_2 Q_2(C_i) - Q_3.$$

Here x is depth and t is time; $C_{i=f,p,d}$ are the component's concentrations; the source terms Q_1 and Q_2 account for the transformations $f \to p$ and $p \to f$ followed by generation and annihilation of the defects, respectively; α_1 and α_2 are constants; and the term Q_3 allows for the defect sinks. Nonlinear dependencies of the sources Q_1 and Q_2 on the concentrations C_f, C_p and C_d provide an appropriate system of feedbacks to describe the spontaneous self-organization. The system of feedbacks is such that 1) the boron clusters precipitation-dissolution recycling, as a whole, generates the defects, and 2) in the presence of the defects the cluster dissolution $p \to f$ slows down. Thus, the defects eventually activate clusterization: local clouds of defects in the presence of boron clusters act like a pump drawing in the surrounding free boron and making it to precipitate into clusters. This results in a self-maintaining growth of large cluster accumulations surrounded by a "dead area" where formation of new clusters is suppressed because of a lack of the free boron. Large groups of clusters formed too close each to another fall into a competition for precipitation and containing of boron. More chances to survive has the largest and densest cluster group, as it produces more of defects which suppress dissolution.

Fig. 1a-d shows an example of numerical modelling of the boron redistribution due to the process of self-organization. It can be seen that the initial smooth depth distribution of boron displayed in Fig. 1a spontaneously splits into six peaks. One of these does not survive the competition with a stronger neighbour and disappears. Finally, a stationary pattern is formed which contains five almost equidistant peaks, as shown in Fig. 1d. In accordance with the experiment [1–3], positions of the main peaks are almost unchanged with time. The distance between the main peaks depends on the diffusion length of free boron and defects. From our model calculations a tentative estimate of the defects diffusion coefficient was obtained, $D_d = 10^{-14} \div 10^{-13}$ cm^2/s.

We are to emphasize that the model used in our work is one-dimensional, while the real system under consideration is three-dimensional, which should be accounted for in

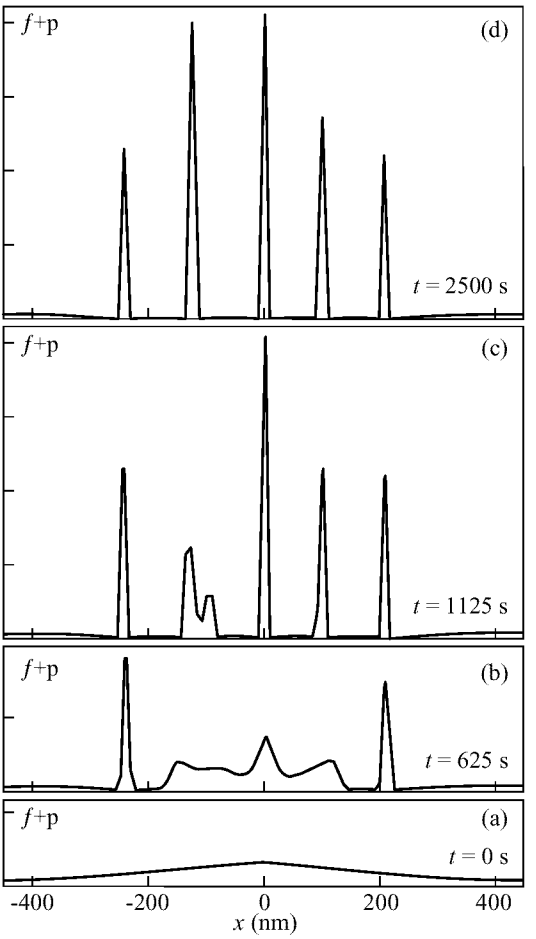

Fig 1. Model depth distributions of boron, $C_f + C_p$, at various stages of the self-organization. (a) an initial model distribution; (d) the final stationary distribution.

the subsequent sophisticated models. However, from the general theory [6] it can be concluded that simple approximate approaches like the present give, as a rule, a good qualitative picture of self-organization processes.

Thus, the simple qualitative "reaction-diffusion" model put forward in this work on the basis of the theory of self-organization [4–6] explains the formation of complex spatial distribution of boron in highly-doped silicon. The model predicts an important role of mobile crystalline defects which are to activate the process of self-organization. The model also allows to estimate the diffusion coefficient of the defects. We do not specify the proposed defects in this work because this requires additional experimental information. New experimental studies of the boron-implanted silicon structure are expected to provide solid grounds for more exact quantitative models of self-organization of boron clusters in silicon.

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