Physica B 407 (2012) 2176–2184

Contents lists available at SciVerse ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Modeling of the transient interstitial diffusion of implanted atoms during low-temperature annealing of silicon substrates

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ARTICLE INFO

Article history:
Received 31 August 2011
Received in revised form
28 January 2012
Accepted 24 February 2012
Available online 3 March 2012

Keywords:
Diffusion
Annealing
Doping effects
Boron
Silicon

ABSTRACT

It has been shown that many of the phenomena related to the formation of "tails" in the low-concentration region of ion-implanted impurity distribution are due to the anomalous diffusion of nonequilibrium impurity interstitials. These phenomena include boron implantation in preamorphized silicon, a "hot" implantation of indium ions, annealing of ion-implanted layers et cetera. In particular, to verify this microscopic mechanism, a simulation of boron redistribution during low-temperature annealing of ion-implanted layers has been carried out under different conditions of transient enhanced diffusion suppression. Due to the good agreement with the experimental data, the values of the average migration length of nonequilibrium impurity interstitials have been obtained. It has been shown that for boron implanted into a silicon layer preamorphized by germanium ions the average migration length of impurity interstitials at the annealing temperature of 800 °C can be reduced from 11 nm to approximately 6 nm due to additional implantation of nitrogen. The further shortening of the average migration length is observed if the processing temperature is reduced to 750 °C. It is also found that for implantation of BF_2 ions into silicon crystal, the value of the average migration length of boron interstitials is equal to 7.2 nm for thermal treatment at a temperature of 800 °C.

1. Introduction

It is well known that boron is a basic impurity of p-conductivity used in the technology of the production of silicon integrated microcircuits [1]. Unfortunately, boron atoms have a small mass and large mobility in silicon crystals. Due to the small masses of boron ions, the formation of an amorphous layer in the ion-implanted substrates is not observed even at large fluencies. Only a great number of radiation defects are created. The absence of an amorphous layer and the presence of radiation defects result in the significant transient enhanced diffusion (TED) of ion-implanted boron during the subsequent annealing (see, for example, [2–20]). All these phenomena substantially complicate the problem of the formation of very shallow junctions with high electrophysical parameters. For suppressing the TED of ion-implanted boron, a method of boron implantation in a silicon layer preamorphized by heavier germanium ions is widely used [9,13–15,21–33]. Due to the solid phase epitaxial regrowth (SPER) of the amorphous layer, the region doped with boron is characterized by a perfect crystal structure, containing defects that are invisible by electron microscopy. However, the transient enhanced diffusion is observed as before, although it has another character and a smaller intensity. In Refs. [34,35] a qualitative difference of the form of boron profiles produced by annealing at temperatures of 800 °C and below was pointed out in comparison with the annealing at 900 °C and higher temperatures. Really, at low annealing temperatures an extended "tail" is observed in the low-concentration region of the impurity profile and the shape of this "tail" is a straight line if the axis of concentration is logarithmic. This feature of the boron distribution is observed even for "tail" extension compared to the characteristic size of the implanted region or smaller than it. At the same time, after annealing at a temperature of 900 °C or higher the shape of the boron profile for concentrations below approximately $10^8\ \mu m^{-3}$ becomes convex upwards, i.e., similar to the Gaussian distribution. This behavior of the profile shape gives clear evidence of the change in the boron diffusion mechanism.

It is worth noting that the "tails" that represent a straight line, if the axis of concentration is logarithmic, are often observed directly after ion implantation of boron, phosphorus, gallium, and other impurity at room temperature (see, for example, Refs. [2,29] in the case of implantation of boron ions, Refs. [36,37] for phosphorus implantation, Refs. [38,39] in the case of implantation of gallium ions). The ion implantation in all the cases investigated was carried out in the direction deflecting from the crystal axis. According to Ref. [40], to completely remove the phenomenon of channeling and to eliminate the "tails" related to the scattering

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doi:10.1016/j.physb.2012.02.036

of ions into channels, the ion implantation should be carried out in amorphous silicon. Nevertheless, later experiments show that "tails" are observed for boron implantation in the layers preamorphized by germanium ions [23,31].

For the low-temperature treatments of ion-implanted layers either an increase and broadening of existing "tails" in the bulk of a semiconductor occur or the formation of new "tails" if they are not observed after implantation. In the region of low impurity concentration, a "tail" represents as before a straight line for low-temperature annealing (i.e., for a small thermal budget). Really, an increase in the "tail" extension occurs during subsequent thermal treatments of preamorphized silicon layers that were implanted with boron ions [23,27,31,32]. In the investigations carried out by Refs. [15,22,28,33] clearly identified "tails" after boron implantation were not observed. However, such "tails" were formed in the course of the subsequent annealing. As follows from the experimental data of Ref. [41], a "tail" is also formed in the case of thermal treatment at 900 °C of silicon layers implanted with indium. This "tail" represents a straight line if the concentration axis is logarithmic. The experimental data also show that "tails" characterized by a straight line are often observed for the "hot" ion implantation of indium [41], gallium [41], antimony [42], and other impurities.

It was assumed originally that the formation of "tails" in the low-concentration region of ion-implanted impurity profiles, especially in the case of "hot" ion implantation, results from the fast diffusion of implanted impurity atoms [38,41–43]. It was supposed that impurity interstitials are this fast diffusing species [41,38,43]. For example, it was shown experimentally in Ref. [43] that during annealing of ion-implanted layers a significant fraction of indium and tellurium atoms leave their substitutional positions and become interstitials. The interstitial position is also a characteristic feature for atoms of gallium that, as well as boron, indium, and tellurium, is the element of III groups. However, in the latest papers [37,39] there are very serious arguments that the formation of "tails" in ion-implanted layers is related to the scattering of ions that reserved a part of the kinetic energy into channels. For example, in Ref. [37] phosphorus ions were implanted into thin silicon layers of different thicknesses. These layers were located on a substrate, which collected ions channeling through the layer. It was assumed that diffusing atoms do not have sufficient energy to leave the silicon crystal, whereas the channeling ions have. Experiments showed that the substrate really collects ions passed through the silicon layer. The doses of the passed ions were obtained as a function of the layer thicknesses. These doses correspond to the doses of phosphorus atoms in the region of the remainder of the "tail" for the investigated depth if ions were implanted in the continuous silicon. The results obtained were generalized in Ref. [39] for the cases of indium and gallium implantation. According to Ref. [39] the radiation-enhanced diffusion of gallium is impossible at room temperature. On the other hand, a characteristic "tail" is observed experimentally due to the scattering of ions into channels. Taking into account the possible annealing of damages and recovery of the crystal structure in the region of the end of the ion range, one can explain the results of Ref. [41] for "hot" high fluence implantation of indium and gallium ions without attracting the concept of an anomalous diffusion. Besides, at low temperatures a "tail" can be formed as a result of the channeling of a part of impurity atoms at the initial stage of implantation, when the amorphous phase was not formed as yet. Nevertheless, the mechanism of the "tail" formation is not clear until now, especially taking into account the latest experiments [23,31] related to boron implantation in the layer preamorphized by implantation of germanium ions. This allows us to formulate the following purpose of the research.

2. Main goal of the research

Not rejecting the possibility for a part of the ions of scattering into channels, we are to show that the long-range migration of nonequilibrium impurity interstitials is the main factor in the formation of "tails" in the region of low impurity concentration for random ion implantation into silicon crystals and implantation into preamorphized silicon layers.

3. Analysis of the mechanisms of the "tail" formation during ion implantation

Let us consider five characteristic cases of the formation of "tails" in the region of impurity concentration decreasing in the bulk of the semiconductor:

(i) "Tail" formation during the subsequent annealing of ion-implanted layers [41,15,22,28,33].
(ii) Formation of "tails" during ion implantation into amorphous silicon [23,31].
(iii) "Tail" formation during SPER of deposited amorphous Si layer doped with boron [44].
(iv) The phenomenon of "tail" formation during "hot" ion implantation [41,42].
(v) Formation of "tails" during ion implantation in the direction deflecting from the axis of the crystal at room temperature of the substrate [2,29,36–39].

It is evident that in the first three cases, there is no phenomenon of channeling and it is possible to explain the formation of "tails" only by the anomalous impurity diffusion. As an example, Fig. 1 presents the calculation of ion-implanted indium redistribution. The indium concentration profile was calculated within the framework of the model for diffusion of impurity interstitials described below. For comparison, the experimental data of Ref. [41] are used. In the work of Gamo et al. [41] the distributions of impurity atoms were obtained by measuring the γ-ray intensities in a combination with the layer removal technique. Indium was implanted with an energy of 45 keV to a dose of $\sim 1 \times 10^{15}$ ion/cm^2 and 8° off the $\langle 111 \rangle$ axis in order to reduce channeling effects. The temperature of annealing was 900 °C, and the thermal treatment duration was 20 min. The following values of parameters for the model of interstitial diffusion of ion-implanted impurity were used. The parameters of the as-implanted indium distribution are: $R_p = 0.03$ μm (30 nm); $\Delta R_p = 0.0084$ μm (8.4 nm); the parameters of the indium interstitial diffusion are: the

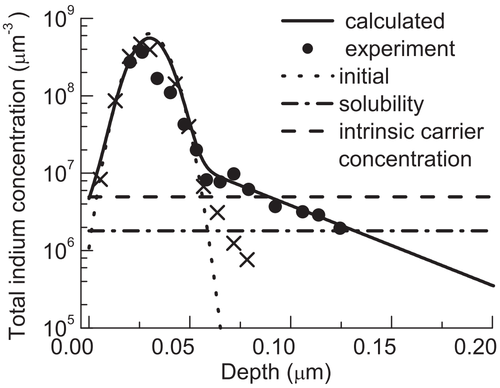

Fig. 1. Calculated indium concentration profile (solid line) after thermal treatment of implanted silicon substrate at 900 °C for 20 min. Gaussian distribution (dotted line) was used to approximate the initial impurity profile. The experimental data (× —impurity distribution after implantation; •—after annealing) are taken from Ref. [41] and the indium solubility limit is taken from Ref. [45].