SIMULATION OF THE INITIAL STAGE OF Si CLUSTER FORMATION UPON POST-IMPLANTATION ANNEALING OF SiO_2

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Abstract

The evolution of the $SiO_{1.7}$ defect structure caused by ion implantation of Si^+ and post-annealing at 1500 K for 100ns has been simulated. Clustering of embedded silicon atoms is detected for the selected ion dose of $1 \cdot 10^{17} cm^{-2}$.

Introduction

Purpose

Estimate the time of relative stabilization of the a-SiO_2 structure during post-implantation annealing

Object of research

Non-stoichiometric amorphous silicon dioxide $SiO_{1.7}$, ion-irradiated Si^+ with energy 20 keV and dose 10^{17} cm^{-2}, annealing temperature T_{ann}=1500K.

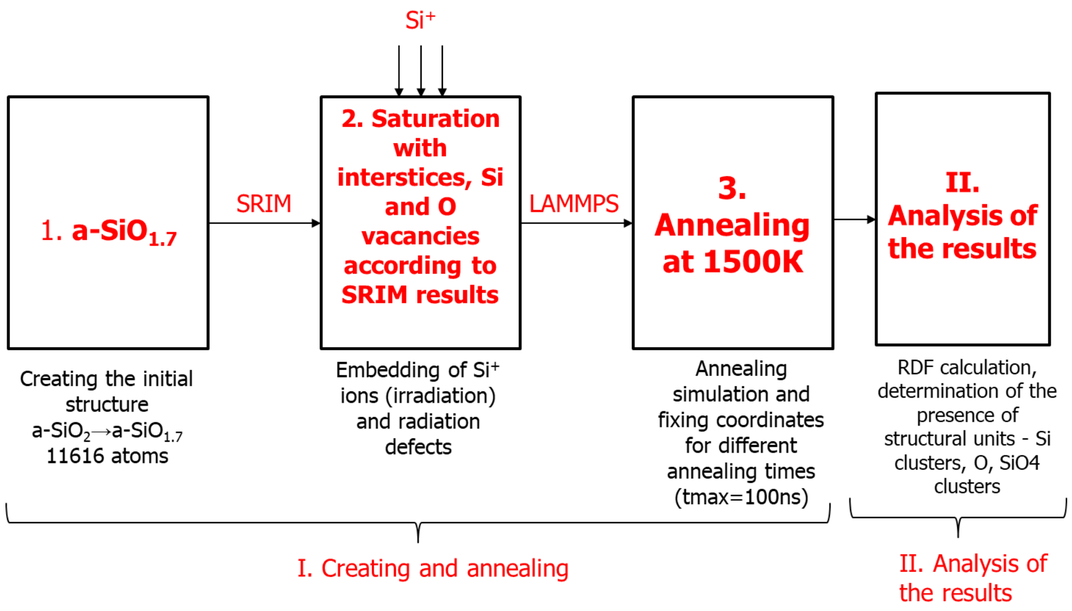
Result

The formation of nanoclusters for a time of 100 ns was found.

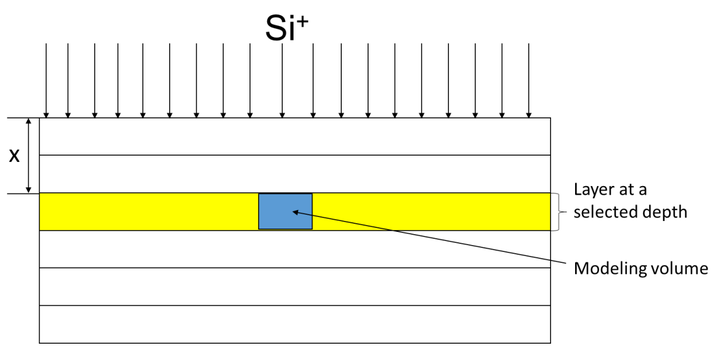
Used tools

A. SRIM
B. LAMMPS
C. Original programs for analyzing the simulated structure at different stages of the study

Simulation Algorithm



Using SRIM

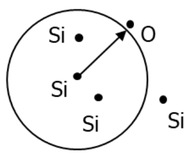


File ***VACANCY*** – concentration of Si and O vacancies
File ***RANGE*** – concentration of displaced Si and O (recoil atoms), number of embedded Si ions at depth x
X = 250A selected in the region of maximum concentration of Si^+ ions for the selected energy

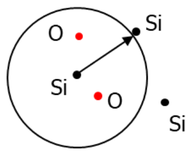
Analysis method and result

Estimation of the type, number and size of structural units in the simulated volume depending on the annealing time

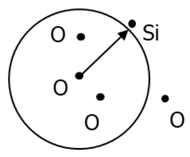
1. Spheres containing only nSi atoms (1,….n)



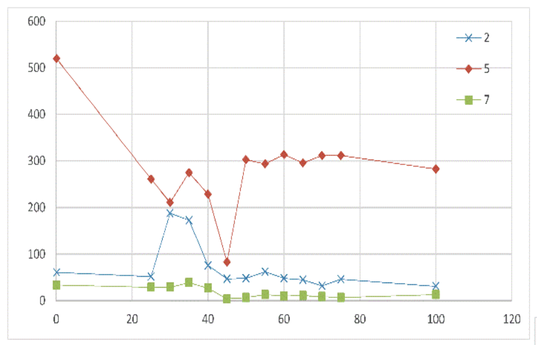
2. Spheres containing one Si atom + (1,….n) atoms O



3. Spheres containing only nO atoms (1,….n)

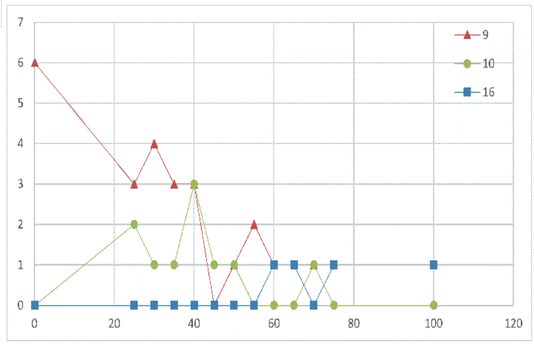


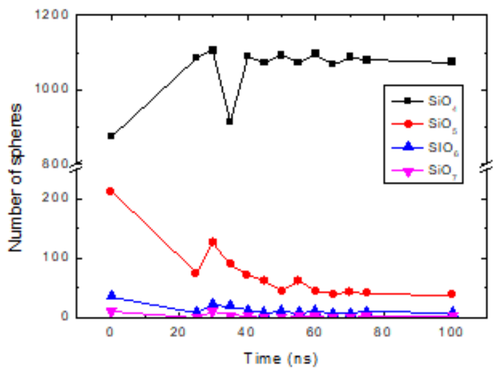
This work was supported by the Government of the Russian Federation (contract № 074-02-2018-330 (2))



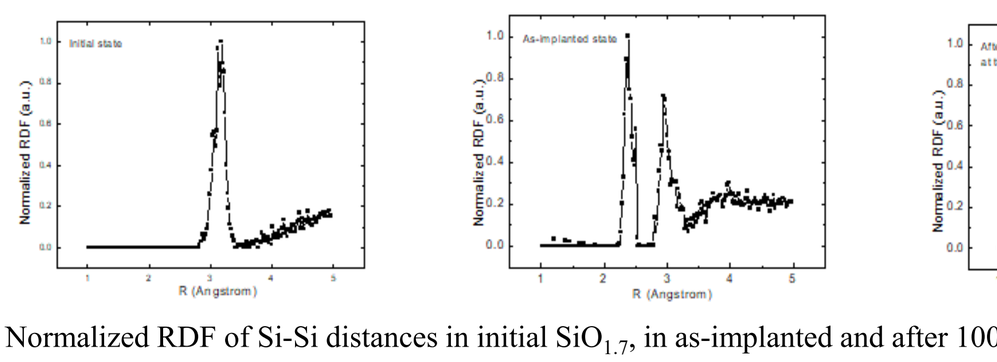
Time dependence of the number of clusters containing different numbers (2, 5, 7, 9, 10, 16) of silicon atoms.

There is a change in the number and size of sphere-clusters

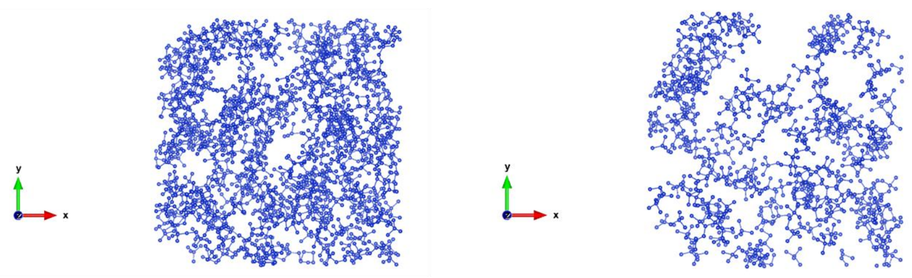




Time dependence of the number of SiO_n components (n = 4, 5, 6, 7)

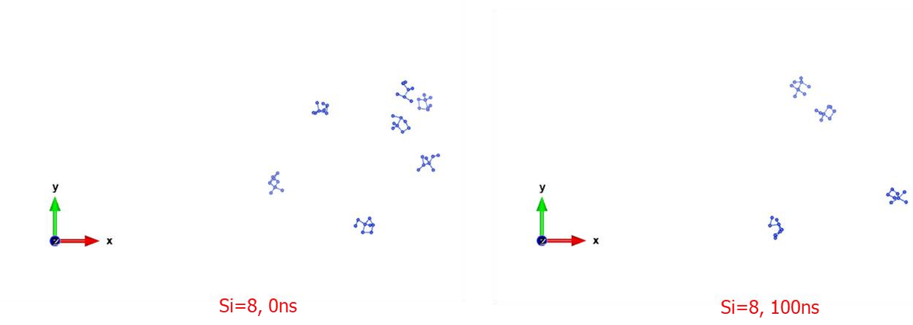


Normalized RDF of Si-Si distances in initial $SiO_{1.7}$, in as-implanted and after 100 ns annealing at 1500K.



Si=5, 0ns

Si=5, 100ns



Si=8, 0ns

Si=8, 100ns

Evolution of clusters depending on the annealing time

Conclusions

The results obtained showed the possibility of evaluating the structure of irradiated amorphous a-SiO_2 at the early stages of post-implantation annealing depending on the temperature and radiation dose. The formation of nuclei of silicon nanoclusters and the restoration of the damaged structure of SiO_2 are found.

The results can be useful for understanding the nature of the effect of irradiation on the stability of characteristics of silicon oxide-based memristors.

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