Diffusion and Deactivation of As in Si: Combining Atomistic and Continuum Simulation Approaches

A. Martinez-Limia[a], C. Steen[b], P. Pichler[a,b], N. Gupta[c], W. Windl[c], S. Paul[d], and W. Lerch[d]

[a] Fraunhofer Institute of Integrated Systems and Device Technology, Schottkystrasse 10, 91058 Erlangen, Germany
alberto.martinez@iisb.fraunhofer.de

[b] Chair of Electron Devices, University Erlangen-Nuremberg, Cauerstrasse 6, 91058 Erlangen, Germany

[c] Department of Materials Science and Engineering, The Ohio State University, 2041 College Road, OH 43210-1178, USA

[d] Mattson Thermal Products GmbH, Daimlerstrasse 10, 89160 Dornstadt, Germany

Abstract

Possible arrangements of As in bulk Si have been investigated using ab initio calculations to establish the most stable configurations depending on As concentration and charge state. Consistently with these results we developed a continuous model for As activation and diffusion in Si. The model was implemented in the Sentaurus Process Simulator and calibrated using a wide range of experimental results available in the literature. It was independently tested for spike and flash annealing experiments with excellent results.

1 Introduction

Arsenic is used as n-type dopant in the present CMOS technology. With decreasing vertical dimensions of the contact regions of the devices, active concentrations around the solubility maximum are required. In order to support process development, it is important to understand the interconnected physical phenomena that govern dopant activation and diffusion. Extrinsic diffusion, precipitation at high concentration, preferred deactivation configurations, segregation processes at the Si/SiO_2 interface, amorphization by implantation, and the activation state after solid phase epitaxy are some of the aspects that are not well established for As in spite of the extensive research work in this direction.

In the first part of this work we present ab initio calculations of basic As configurations in bulk Si to find the most stable structures depending on As concentration and charge state. In the second part we present a continuous model for As activation and diffusion in Si where we have implemented the fundamental physical processes involved. The model was developed in consistence with the results of our ab initio simulations and has been tested for a wide range of As annealing experiments.

2 Ab initio calculations

We performed ab initio calculations of six model structures of As in Si (Fig. 1) using the plane-wave density functional theory code VASP with ultra soft pseudopotentials within the generalized gradient approximation. These structures are representative of possible As configurations discussed in the literature [1, 2]. Periodic boundary conditions and cell sizes adapted to the models were used. The calculations were done for charges of 0, +1, +2, +3, and +n (n being the number of As atoms in the system; +n means that all As atoms are electrically active). For all six configurations, either 0 or +n had the lowest energy (expressed by the calculated chemical potential of As). Fig. 2 shows a summary of our results.

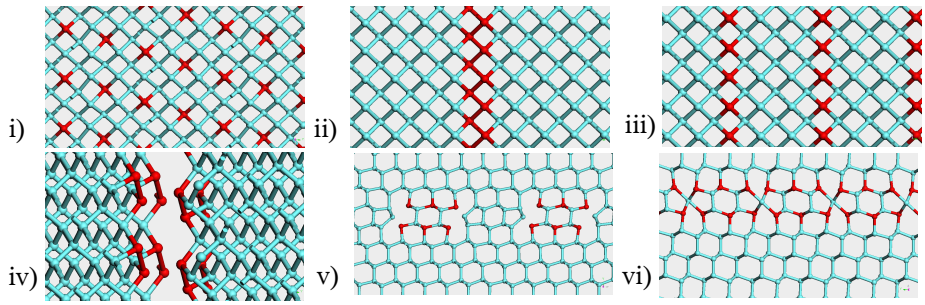

Figure 1: Three dimensional configurations of As (red atoms) in Si (blue atoms). i) As atoms uniformly distributed, ii) two As monolayers next to each other, iii) two As monolayers separated from each other, iv) As surface-like reconstruction with threefold coordinated configurations, v) small SiAs arrangement, and vi) SiAs layer.

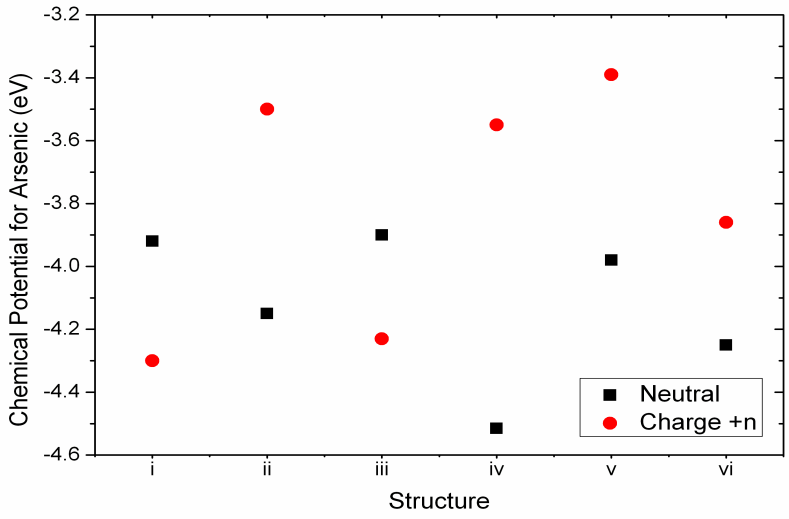

Figure 2: Chemical potential of active and neutral As for the structures of Fig. 1.

The results demonstrate that full activation (+n charged system) can only be achieved if all As atoms have four Si neighbors ((i) and (iii)), where uniformly distributed As (i) is more favorable due to the minimization of Coulomb repulsion. In contrast, As-As bonds ((ii) and (iv)) as well as an As coordination similar to that found in SiAs precipitates ((v) and (vi)) result in complete deactivation. The lowest-energy configuration (iv) was obtained after energetic relaxation of (ii), resulting in threefold coordinated As and complete deactivation. A similar deactivating configuration can also be expected at surfaces, Si/SiO_2 interfaces, or in As_nV clusters. Small neutral SiAs clusters (v) are not favorable, in contrast to whole SiAs layers (vi), or larger precipitates, that should be the preferable inactive configuration for high As concentrations.

3 Diffusion and activation model

Taking into account our ab initio results, we have developed a diffusion and activation model for As. The model includes for the first time the simultaneous formation of arsenic-vacancy (As_4V) complexes and the precipitation of a SiAs phase. The latter is mandatory to correctly describe concentrations above solid solubility while the former are needed to describe the reduced electrical activity as well as the generation of self-interstitials during deactivation. A segregation model at the Si/SiO_2 interface including arsenic deactivation, consistent with our ab initio results, is taken into account.
The model was implemented into the latest version of the Sentaurus Process Simulator of Synopsys and optimized using about 15 reported series of diffusion coefficients for temperatures between 700 °C and 1200 °C, and 28 SIMS profiles covering annealing processes from spike to very long times with temperatures between 700 °C and 1050 °C and a wide distribution of implantation energies and doses. As an example, Fig. 3 shows the simulations of an experiment reported by Solmi and Ferri [3]. The excellent agreement between experiment and simulation is apparent.

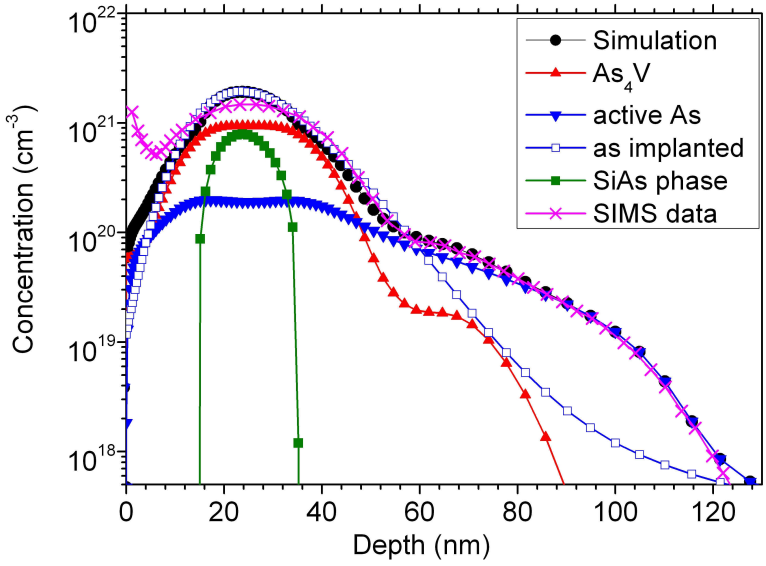

Figure 3: SIMS As profile for a sample implanted with 35 keV, 5×10^{15} cm^{-2} As, annealed at 750 °C for 30 min [3], together with our simulation.

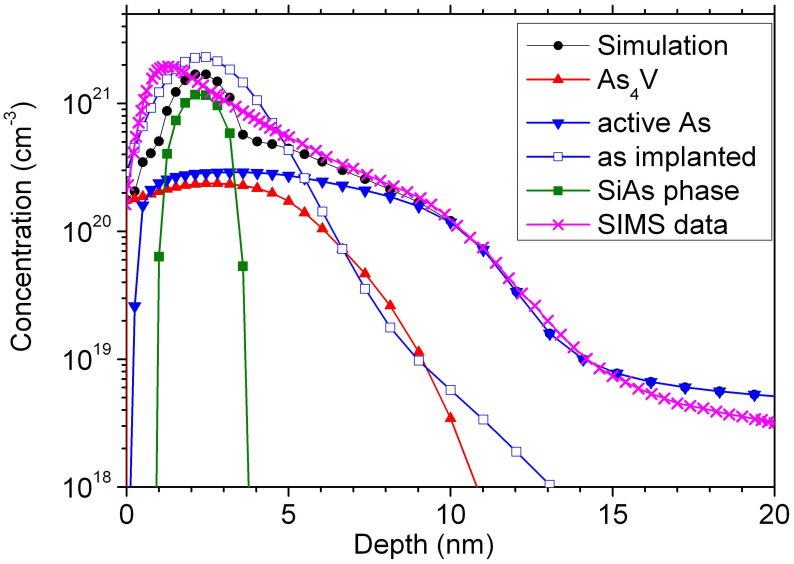

Figure 4: SIMS As profile for a sample implanted with 1 keV, 1×10^{15} cm^{-2} As, spike annealed at 1000 °C at Mattson Thermal Products GmbH, and our simulation.

To validate our model we performed simulations of spike and flash annealing experiments done at Mattson for temperatures in the range from 1000 °C to 1300 °C. We were able to reproduce with good accuracy shape of the annealed profiles and the active dose determined by Hall measurements. Fig. 4 shows the results of one of the simulations. A detailed discussion of these experiments is published elsewhere [4].

Acknowledgments

This work has been funded by the European Union (IST project 027152 ATOMICS), the National Science Foundation (contract No. 0244724), the Semiconductor Research Corporation (contract No. 2002-MJ-1018), and the Deutsche Forschungsgemeinschaft (contract No. Ry 1/23). WW acknowledges support from the Fraunhofer Society and Humboldt Foundation within a Fraunhofer-Bessel fellowship.

References

[1] F. Iacona, V. Raineri, and F. La Via, Arsenic redistribution at the SiO_2/Si interface during oxidation of implanted silicon, Phys. Rev. B 58, 10990 (1998).

[2] J. Dabrowski, H.-J. Müssig, V. Zavodinsky, R. Baierle, and M. J. Caldas, Mechanism of dopant segregation to SiO_2/Si (100) interfaces, Phys. Rev. B 65, 245305 (2002).

[3] S. Solmi and M. Ferri, Transient enhanced diffusion of arsenic in silicon, J. Appl. Phys. 94, 4950 (2003).

[4] W. Lerch, S. Paul, J. Chan, S. McCoy, J. Gelpey, F. Cristiano, F. Severac, P. F. Fazzini, D. Bolze, P. Pichler, A. Martinez, A. Mineji, and S. Shishiguchi, Experimental and theoretical results of dopant activation by a combination of spike and flash annealing, International Workshop on Junction Technology, IWJT '07 (2007).