O46 | **Positron probing of open vacancy volume of a thermally stable phosphorus-vacancy complex in electron-irradiated silicon**

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We will discuss theoretical and experimental data related to a microstructure of the phosphorus-vacancy complex which has been elusive from observation for decades in float zone silicon single crystals, n–FZ–Si(P). A surprising behaviour of the positron lifetime was investigated in the course of annealing of material irradiated by 0.9-MeV electrons. It turns out that a well-known procedure of isochronal annealing of irradiated wafers for restoring the electrical activity of the phosphorus dopant by decomposing the phosphorus-vacancy pairs of radiation origin (so-called E–centers) is far from perfection: a considerable amount of the impurity atoms of phosphorus are remaining inactive as the shallow donors in the course of isochronal annealing from ~ 100 °C to ~175 °C. A new approach is needed because much higher annealing temperatures are required for restoring electrical parameters of the irradiated material which is of paramount importance for the semiconductor technology.

To gain insight into microstructure of thermally stable radiation centers suppressing electrical activity of the phosphorus dopant we have investigated their isochronal annealing.

The decomposing of these centers was found to begin at ~ 300 ºC [1]. The defect-related long positron lifetime τ_2 ~ 278 ps is steady up to the limit of its reliable detecting at the annealing temperature ~ 500 ºC; the average positron lifetime τ_{av} just approaches to the value 216 ps characteristic of the non-irradiated material.

These data correlate with the ones of low-temperature Hall effect measurements demonstrating for the same material that the isochronal annealing is complex. Three stages were found for recovery of the concentration of charge carriers and mobility [2]: ~ 100 ºC – 180 ºC, ~ 200 ºC – 300 ºC, and at ~ 600 ºC – 650ºC the annealing is accomplished.
It is argued that the thermally stable defects are the phosphorus-vacancy complexes, P–V_{op}. The open vacancy volume V_{op} to be characterized by long positron lifetime τ_2 ~ 278 ps in P–V_{op} complex is compared with theoretical data available for the vacancies and divacancies.

The extended semi-vacancies, 2$V_{s\text{-}ext}$, and relaxed vacancies, 2V_{inw}, are proposed as the open volume V_{op}. It is suggested that larger number of P–Si bonds (at least, five; PSi_5) in the microstructure $V_{s\text{-}ext}$ –P–$V_{s\text{-}ext}$ underlies its high thermal stability. In this case the open volume V_{op} is equal to 2$V_{s\text{-}ext}$ and $V_{s\text{-}ext}$–P–$V_{s\text{-}ext}$ complex possesses a distorted D_{3d} (or O_h) symmetry. In the light these data, a necessity of reconsideration of the whole conception of formation of the positron-sensitive phosphorus-vacancy complexes in silicon is shortly discussed.

[1] N. Arutyunov, V.Emtsev, R. Krause-Rehberg , M. Elsayed, G. Oganesyan, and V. Kozlovski, *Phys. Stat. Sol. (c)*, 13, 807 (2016)
[2] V.V. Emtsev, N.V. Abrosimov, V.V. Kozlovski, G.A. Oganesyan, and D.S. Poloskin, *Semiconductors* 50, 1291 (2016).@ Pleiades Publishing Ltd., 2016