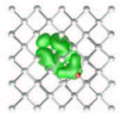
Dislocations and vacancy clusters in silicon deformed at different temperatures

H. S. Leipner, Z. Wang, H. Gu, V. Bondarenko, R. Krause-Rehberg, J. L. Demenet, J. Rabier

Martin-Luther-Universität Halle–Wittenberg,
Wuhan University, Université de Poitiers



PSSD-2002
Sendai

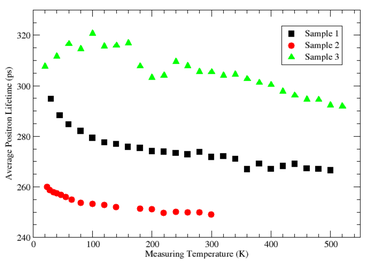
Experiment

- Float-zone silicon, P-doped (samples 1, 2, 3)
- Samples 1 and 2 were dynamically deformed in single-slip orientation under application of a 5 GPa confining pressure in an anisotropic multi-anvil apparatus at room temperature and 150 °C. The deformation rate was 5×10^{-5} s^{-1}.
- Sample 3 was deformed with a constant strain rate of 2.2×10^{-5} s^{-1} under low applied stress from 0 to 20 MPa at 850 °C.
- Sample 1 was strained up to 16 %, sample 2 up to 9 %, sample 3 up to 7 %.
- Conventional fast–fast positron lifetime. FWHM = 260 ps
- Isochronal annealing up to 1300 °C in vacuum

Microstructure after RT deformation

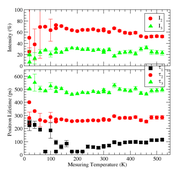
- High number of small cracks are formed in the early stage of the deformation–pressurization. Their extension is stopped when the pressure increase.
- The cracks provide sources for dislocation nucleation and dislocations are emitted from the free surface of cracks.
- The density of dislocations is inhomogeneous. At some cracks dislocation nucleation is not observed.
- Dislocations are undissociated. The plastic deformation at high stress is controlled by perfect shuffle-set dislocations.
- Such dislocations are mainly aligned in ⟨110⟩ orientations (screw dislocations), as well as in ⟨112⟩ orientations (30° dislocations) and in ⟨132⟩ directions (41° between the Burgers vector and dislocation line). The occurrence of these Peierls valleys confirms that different dislocation core configurations appear when dislocations are nucleated at very high stress.

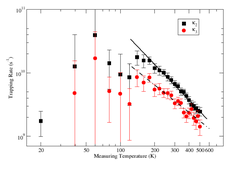
As-deformed state



In all samples, a distinct increase in the average positron lifetime was obtained in comparison with as-grown Si material. In samples 1 and 2, the lifetime increased with the reduction of the sample temperature in the whole temperature range measured, and no saturation appeared at low temperatures. In sample 3, a saturation of the average positron lifetime was observed at low sample temperatures. It can be explained by the presence of shallow positron traps.
The significantly lower average lifetime of sample 2 compared to sample 1 is mainly due to the lower strain.

Sample 3 deformed at 800 °C



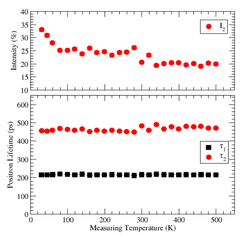


τ_2 is almost independent of the sample temperature with a value of about 500 ps. It is related to larger vacancy clusters. τ_3 amounts to about 280 ps. It can be attributed to positron annihilation in dislocation-bound vacancies.

The trapping rates obtained from a three-state trapping model follow the relations $\kappa_2 \propto T^{-1.8}$ (for the dislocation-bound vacancies) and $\kappa_3 \propto T^{-1.5}$ (for the voids) at temperatures higher than 160 K.

V_{100} ?

Sample 1 deformed at room temperature

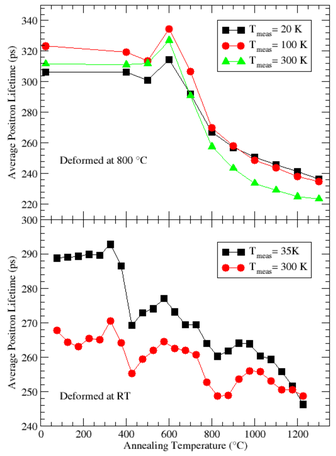


Only two lifetime components can be decomposed. Both lifetime components are independent of the sample temperature. τ_1 is near to the bulk lifetime (218 ps) of as-grown Si. The lifetime τ_2 of about 460 ps is related to larger vacancy clusters. The positron lifetime related to dislocation-bound vacancies found after high-temperature deformation has not been observed after RT deformation.

V_{18} ?

Annealing

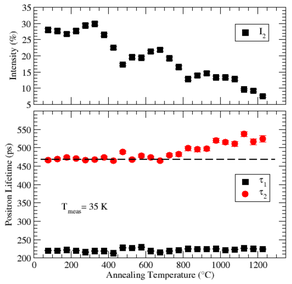
Average positron lifetime



The average positron lifetime is shown for sample 1 deformed at RT and for sample 3 deformed at 800 °C as a function of the annealing temperature after isochronal annealing. The measurements have been carried out at room temperature and at 100 or 35 K. A first drop appears at about 400 °C in both samples. Then the average lifetime increases with the temperature increasing and a maximum is found at the temperature of 600 °C. Another maximum appears after annealing at 1000 °C in sample 1, but not in sample 3. Some defects still remain after annealing at 1200 °C in both samples.

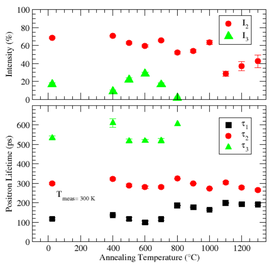
Lifetime components

Sample 1 deformed at room temperature



Positron lifetimes τ_1, τ_2 and intensities I_1, I_2 of sample 1 as a function of the annealing temperature. τ_1 is almost constant and close to the bulk lifetime of as-grown Si. τ_2 increases from 460 ps after 800 °C to 530 ps after 1227 °C annealing.

Sample 3 deformed at 800 °C



Positron lifetime components τ_1, τ_2, τ_3 and intensities I_2, I_3 of sample 3 as a function of the annealing temperature. All lifetimes are independent of the sample temperature during measurement. The lifetime τ_3 for vacancy clusters disappeared after annealing at 800 °C.

Conclusions

- Two types of positron trapping centers related to larger vacancy clusters (lifetime 500 ps) and dislocation-bound vacancies (lifetime 260 to 300 ps) are introduced during deformation at 800 °C. The vacancies on the dislocation line act as deep positron traps, while the regular dislocation line is active as a shallow positron trap. After annealing at 800 °C, the positron trapping centers related to vacancy clusters disappeared, while dislocation-bound vacancies remain.
- Regular dislocation segments (i. e. shallow positron traps) have a significant influence on positron trapping at low temperatures only in samples deformed at high temperatures.
- The only positron trapping centers observed in the samples deformed at RT are related to vacancy clusters (lifetime 460 ps). In contrast to high-temperature deformation, a void-related positron lifetime appears even after annealing at 1227 °C. It increases from 480 ps after annealing at 800 °C to 530 ps after annealing at 1227 °C.
- The different void-related lifetimes found after deformation at 20 and 800 °C may be interpreted by different sizes of the voids. The smaller size after RT deformation may be related in turn to the lower mobility of dislocations in the glide set, provided the dislocation jog dragging is the dominating mechanism of vacancy supply.
- We previously assumed an increase in the density of voids upon annealing leading to the maximum in the average lifetime around 600 °C. However, this simple interpretation fails with the complicated annealing behavior of sample 1 deformed at room temperature.
- A different core structure may be responsible for the findings that in high-temperature deformed Si dislocations act as combined traps (i. e. a regular dislocation lines as shallow positron traps and dislocation-bound vacancies as deep traps), while no dislocation-related trapping is found in the sample deformed at RT.
- The specific lifetime components in sample 1 can be interpreted by an inhomogeneous distribution of positron traps: i) regions of a very high density of traps near cracks and ii) regions almost free of positron traps.

leipner@cmat.uni-halle.de, http://www.cmat.uni-halle.de