Open-volume defects in plastically deformed semiconductors

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Introduction

- Evidence of the formation of point defects during plastic deformation
- What can we learn from positron lifetime spectroscopy (POLIS) about the structure of the defects?
- Theoretical calculation of defect-related positron lifetimes in conjunction with considerations about the stability of various vacancy clusters
- Model of point defect generation
**POLIS results (room temperature)**

### Plastically deformed Si

- \( \tau_{d1} = (285 \pm 20) \) ps
- \( \tau_{d2} = (485 \pm 30) \) ps

### Plastically deformed GaAs

- \( \tau_{d1} = (260 \pm 5) \) ps
- \( \tau_{d2} = (477 \pm 20) \) ps

**d1:** Monovacancy-size defect  \( \Rightarrow \) vacancy in the dislocation core

**d2:** Size \( \gg \) divacancy
Total energy calculations in GaAs

Energy gained by adding a divacancy to an aggregate of \( n - 2 \) vacancies in GaAs (upper part) and the corresponding positron lifetime (lower part). Open/closed symbols: configuration before/after relaxation.
Results of calculations

• Especially stable structures \( (n < 18) \): \( V_6, V_{10}, V_{14} \) in Si
  \( V_{12} \) in GaAs

• Vacancy chains are no energetically favored structures

• Experimentally observed long positron lifetime may be attributed to \( V_{14} \) in Si and \( V_{12} \) in GaAs

• Magic numbers in silicon \( n = 4i + 2, i = 1, 2, 3, \ldots \)

See also Poster of Staab et al.
Formation of vacancy clusters

Agglomeration of vacancies in the wake of the climbing jog

Concentration:
\[ c = \frac{1}{\Omega} \frac{\mathbf{\hat{u}}_1 \cdot \mathbf{u} \times \mathbf{\hat{u}}_2}{|\mathbf{\hat{u}}_1 \cdot \mathbf{u} \times \mathbf{\hat{u}}_2|} \mathbf{b} \cdot \mathbf{u} \times \mathbf{b} \]
Average positron lifetime as a function of the sample temperature. Sample A: undeformed, B: 0.5 % compression, C: 3 % compression. Deformation temperature 625 °C, strain rate $5 \times 10^{-4}$ s$^{-1}$, compression axis [213].
Bistability of positron lifetime

Average positron lifetime measured in plastically deformed undoped GaAs around 100 K upon cooling or heating
Recovery of the average positron lifetime

Average positron lifetime in deformed GaAs as function of the annealing time. The measurement temperature corresponds to the annealing temperature.
DX-like behavior of dislocation-related defects?

- DX centers exhibit a large Stokes shift upon thermally activated electron capture
- DX-like center generated by uniaxial strain field of screw dislocations discovered in DLTS [Istratov, Vyvenko 1996]

- Strain field effect
- Evidence of a metastable behavior in FTIR measurements
- Effect of illumination??
- Electrical measurements
Summary

- Formation of point defects during plastic deformation of semiconductors can be related to the dislocation motion.
- Basic mechanism of emission/absorption of vacancies and interstitials by screw dislocations containing jogs.
- Formation of long rows of vacancies is energetically unfavorable.
- Stable three-dimensional vacancy agglomerates are formed in a primary process by atomic re-arrangement directly at the climbing jog.