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# Open-volume defects in plastically deformed semiconductors

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# Introduction

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- ◆ 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

$$\tau_{d1} = (285 \pm 20) \text{ ps}$$

$$\tau_{d2} = (485 \pm 30) \text{ ps}$$

## Plastically deformed GaAs

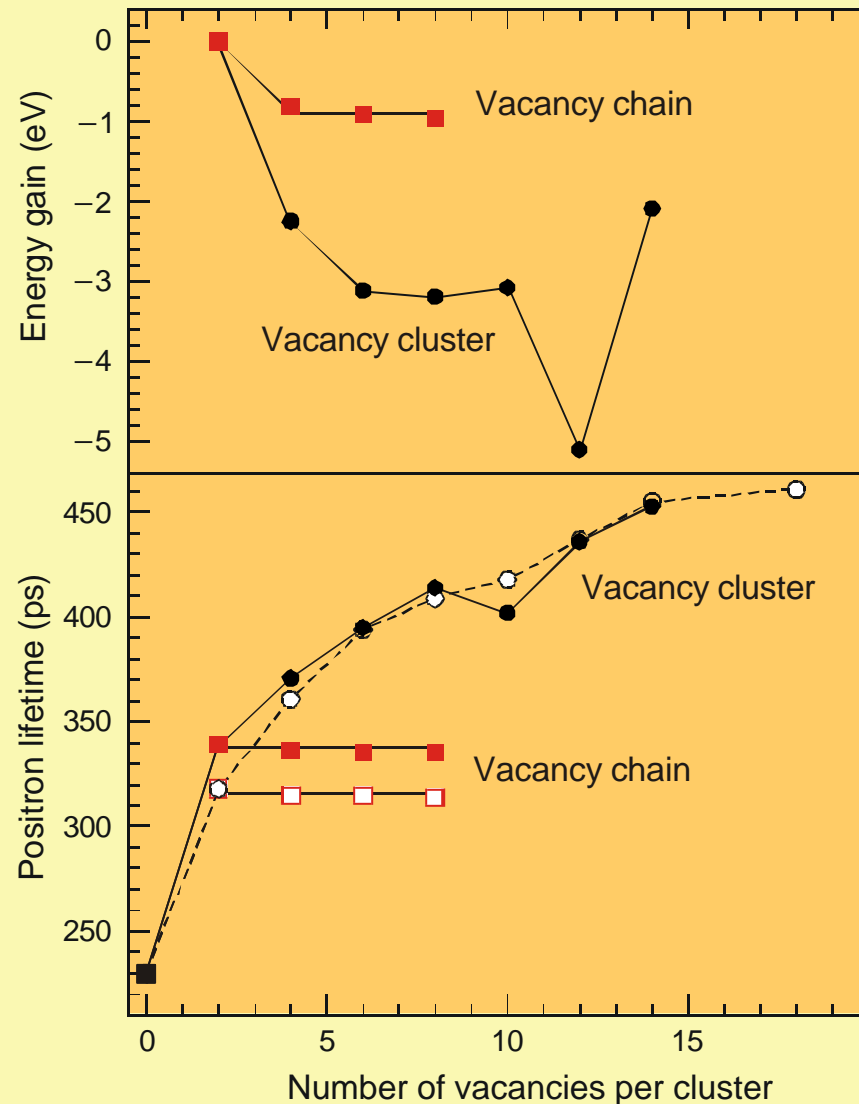
$$\tau_{d1} = (260 \pm 5) \text{ ps}$$

$$\tau_{d2} = (477 \pm 20) \text{ ps}$$

d1: Monovacancy-size defect  $\Rightarrow$  vacancy in the dislocation core

d2: Size  $\gg$  divacancy

# Total energy calculations in GaAs



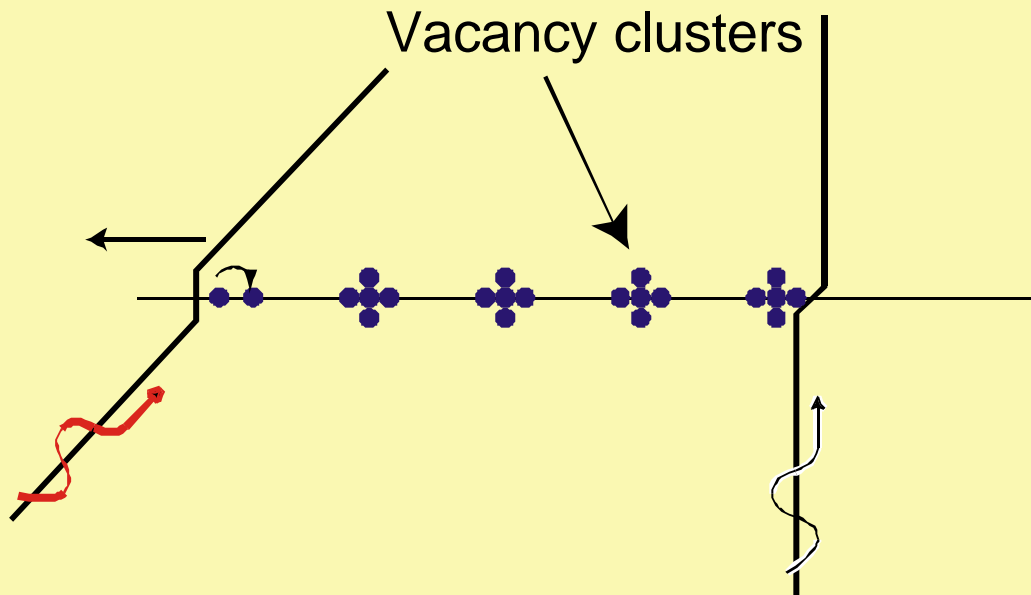
Energy gained by adding a divacancy to an aggregate of  $n - 2$  vacancies in GaAs (*upper part*) and the corresponding positron lifetime (*lower part*). Open/closed symbols: configuration before/after relaxation.

# 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  $n = 4i + 2, i = 1, 2, 3, \dots$

*See also Poster of Staab et al.*

# Formation of vacancy clusters

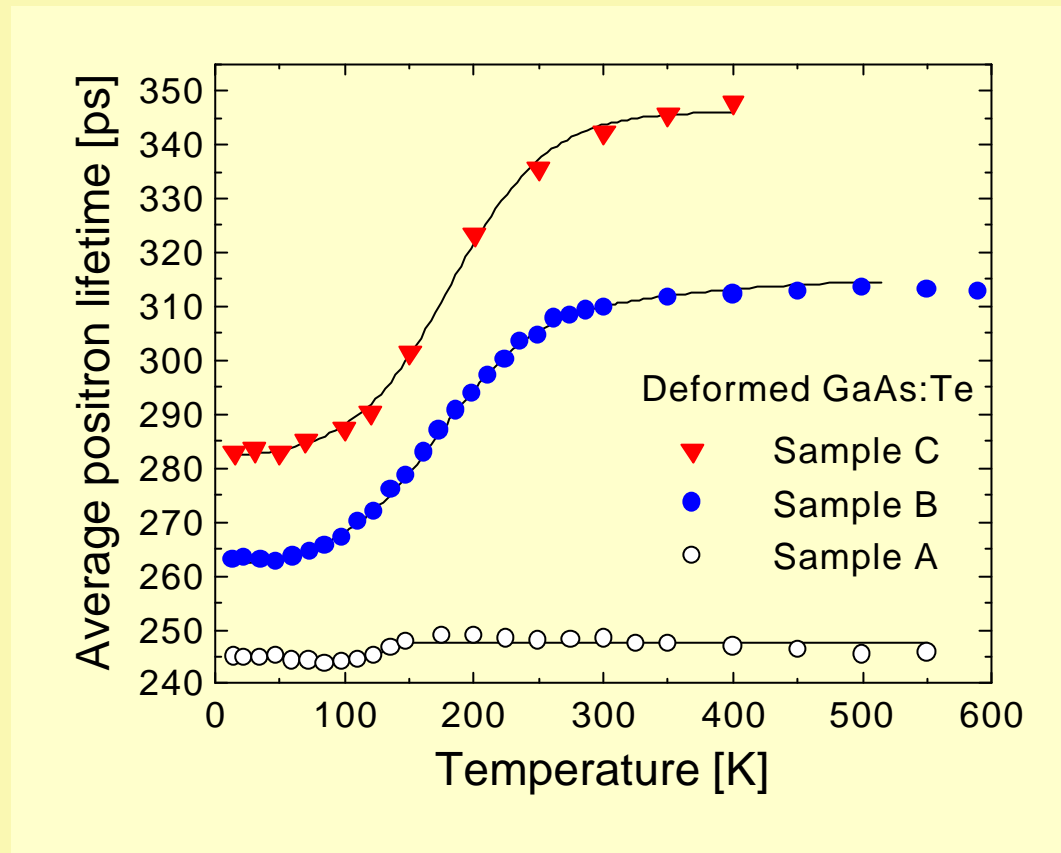


**Concentration:**

$$c = \frac{1}{\Omega} \frac{\hat{\mathbf{i}}_1 \cdot \mathbf{u} \times \hat{\mathbf{i}}_2}{|\hat{\mathbf{i}}_1 \cdot \mathbf{u} \times \hat{\mathbf{i}}_2|} \mathbf{b}_1 \cdot \mathbf{u} \times \mathbf{b}_2$$

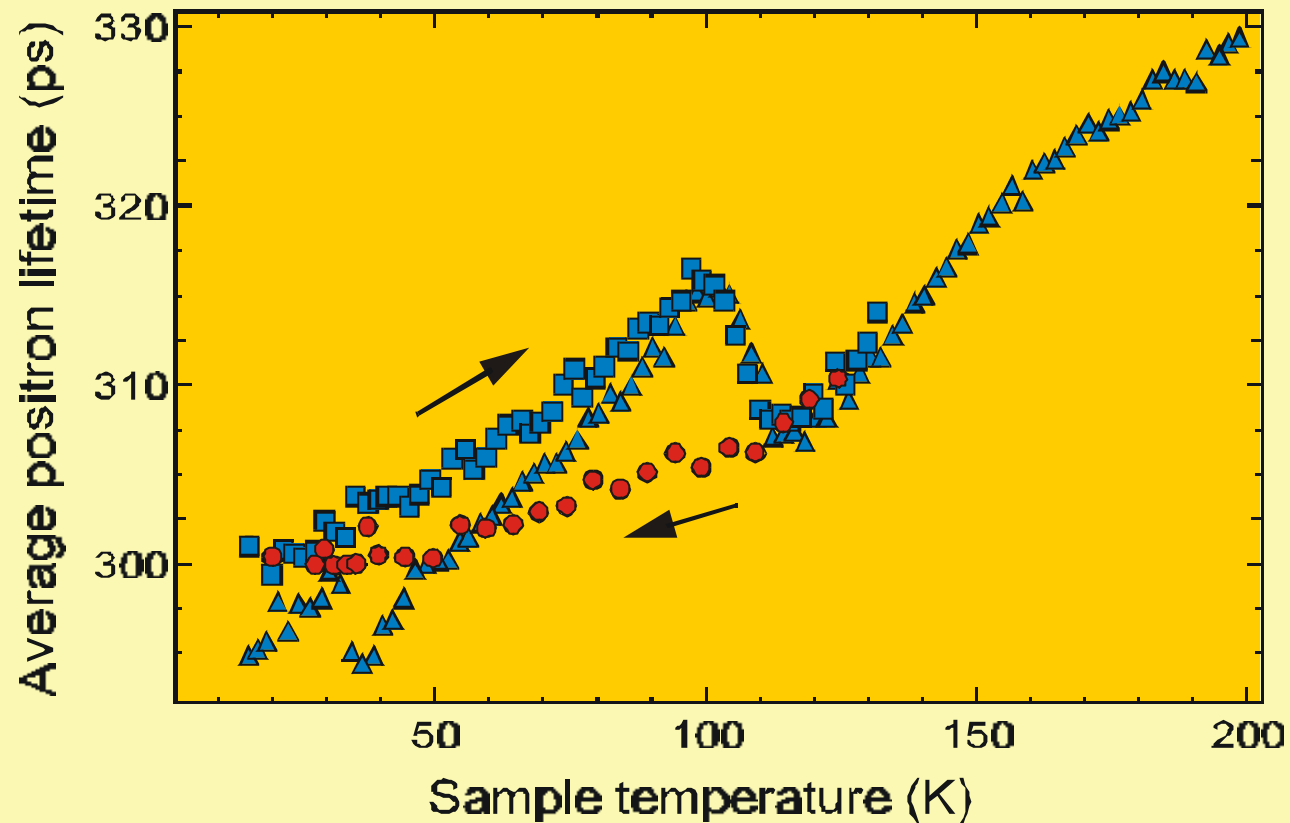
Agglomeration of vacancies in the wake of the climbing jog

# Positron lifetime in plastically deformed GaAs



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  $5 \times 10^{-4} \text{ s}^{-1}$ , compression axis [213].

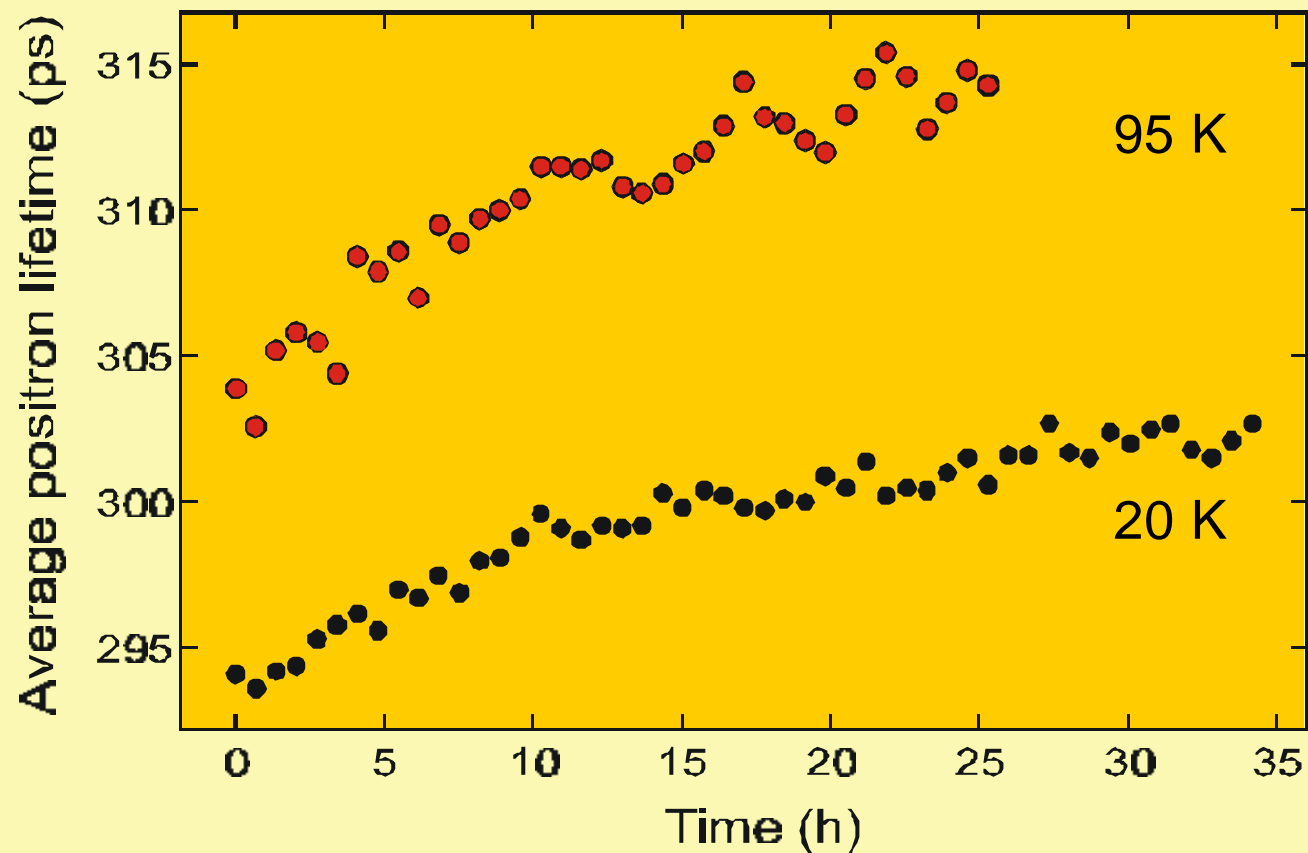
# Bistability of positron lifetime



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