Characterization of defects in Ni alloys based on gamma-ray-induced positron annihilation lifetime spectroscopy at UVSOR

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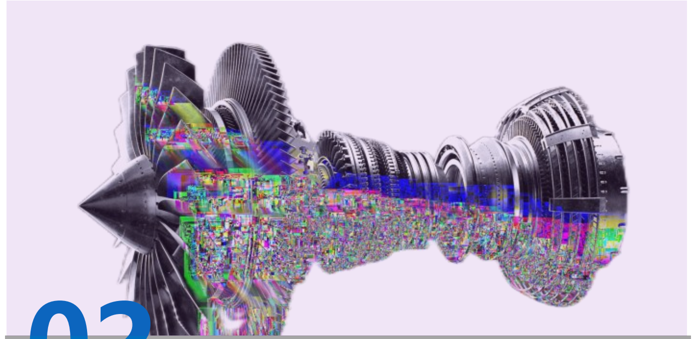
OUTLINE

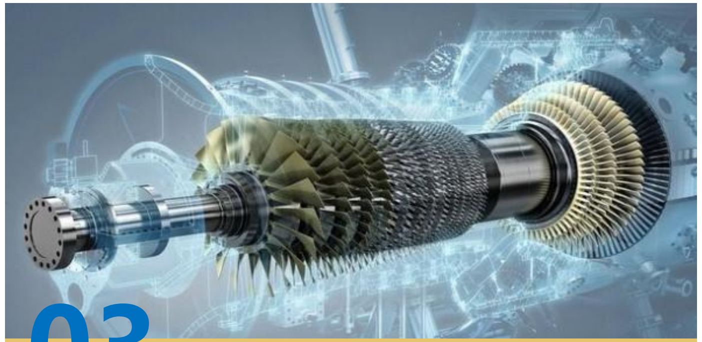
- Research motivation
- Experimental method
- Results
- Conclusions

MOTIVATION

01 Nuclear energy



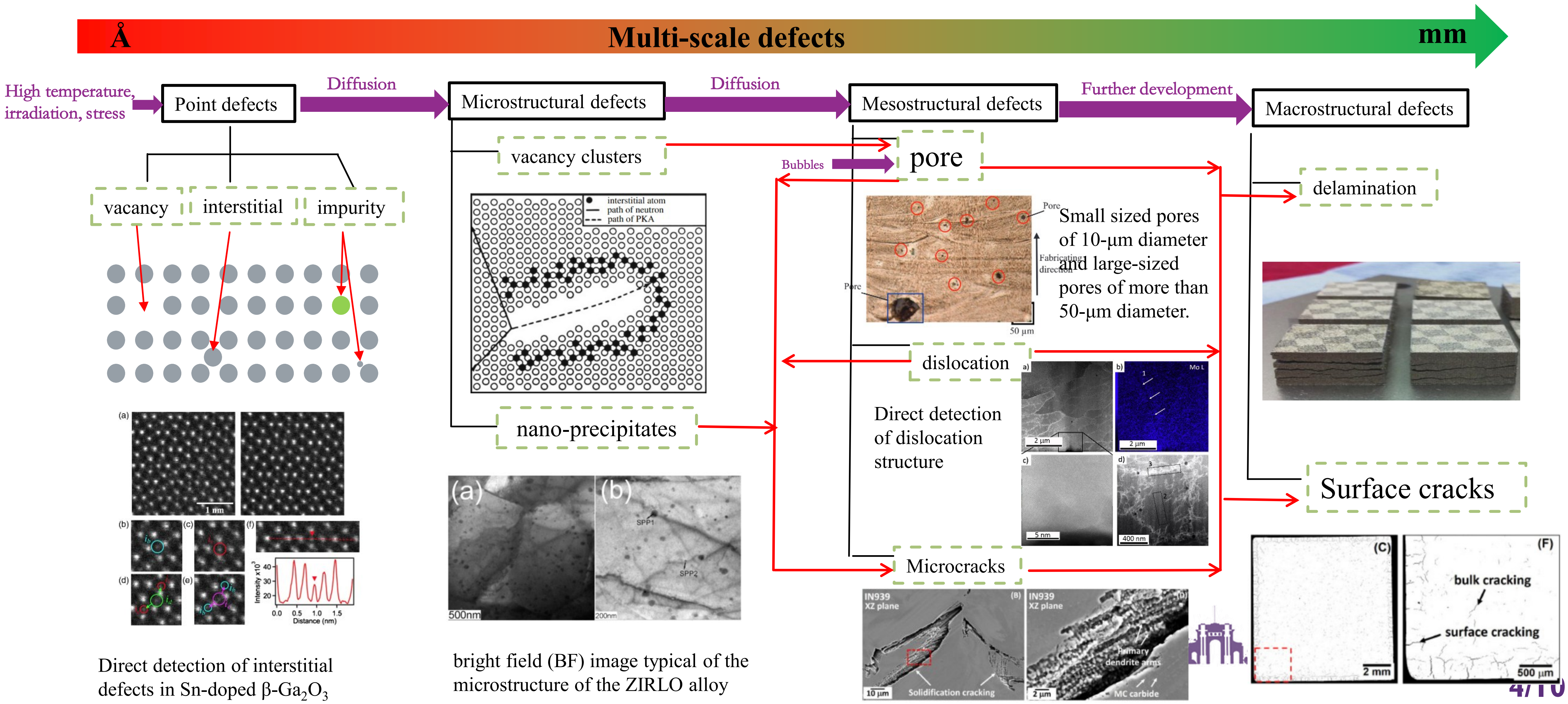
02 aero-engine



03 gas turbine

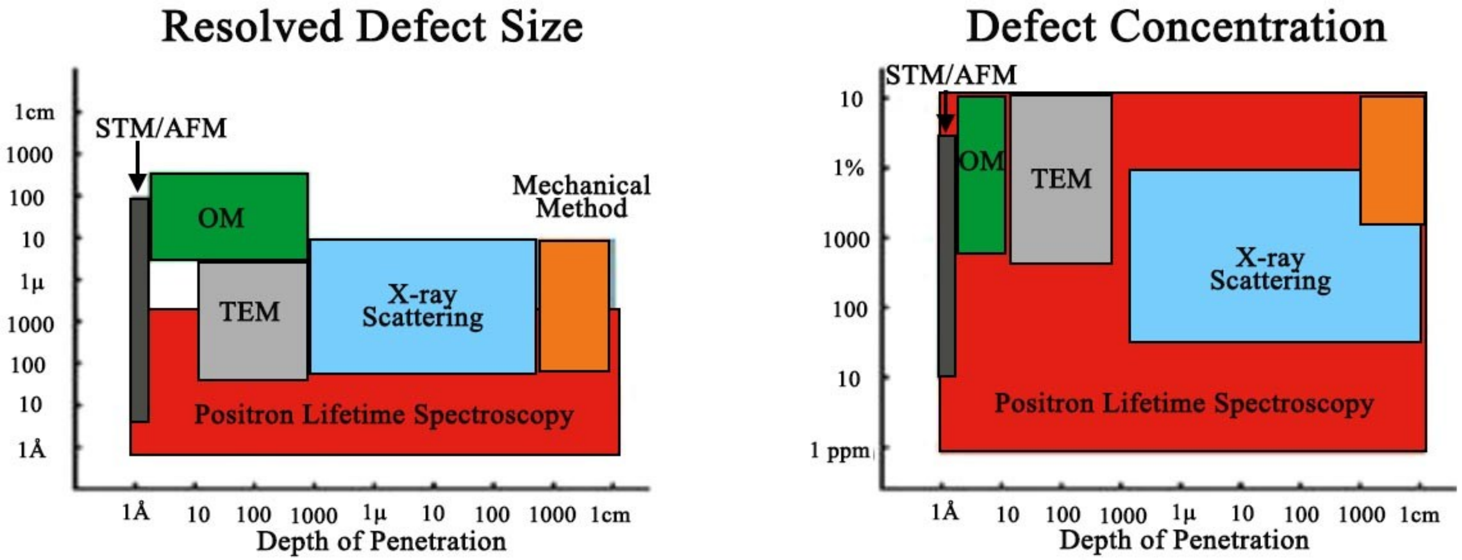
Nickel based superalloys are widely used in various industrial applications, particularly in the hot sections, like nuclear energy installations, aero-engines, gas turbines, and other critical equipment. However, during long-term service under cyclic mechanical and thermal load, the stability of the superalloys may deteriorate as the formation of microscopic defects.

MOTIVATION


Å
Multi-scale defects
mm
High temperature, irradiation, stress
Point defects
Diffusion
Microstructural defects
Diffusion
Mesostructural defects
Further development
Macrostructural defects
vacancy
interstitial
impurity
vacancy clusters
interstitial atom
path of neutron
path of PKA
nano-precipitates
Bubbles
pore
Pore
Small sized pores of 10-μm diameter and large-sized pores of more than 50-μm diameter.
50 μm
dislocation
Direct detection of dislocation structure
2 μm
5 nm
400 nm
Microcracks
IN939 XZ plane
Solidification cracking
Primary dendrite arms
MC carbide
10 μm
2 μm
delamination
Surface cracks
bulk cracking
surface cracking
2 mm
500 μm
1 nm
Intensity x10^3
Distance (nm)
500nm
200nm
SPP1
SPP2
Direct detection of interstitial defects in Sn-doped β-Ga_2O_3
bright field (BF) image typical of the microstructure of the ZIRLO alloy

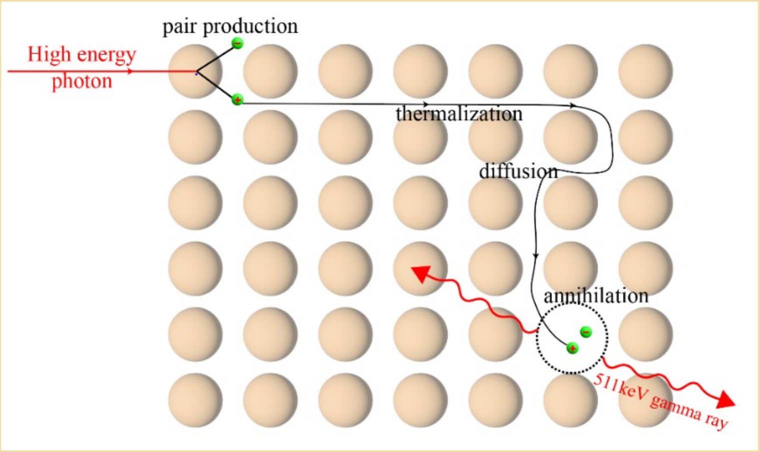
MOTIVATION

Characterization of defects with nanoscale microstructure is essential for accurately assessing the remaining service life.



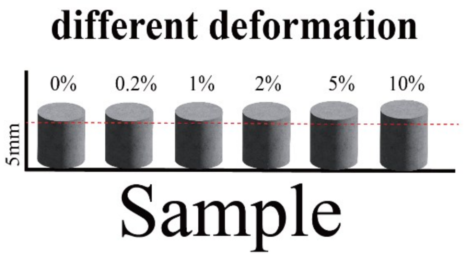
Comparison of the sensitivity of various techniques in defect measurements with respect to depth, size and concentration.

TEM: transmission electron microscopy,
STM: scanning tunneling microscopy,
AFM: atomic force microscopy,
OM: optical microscopy,

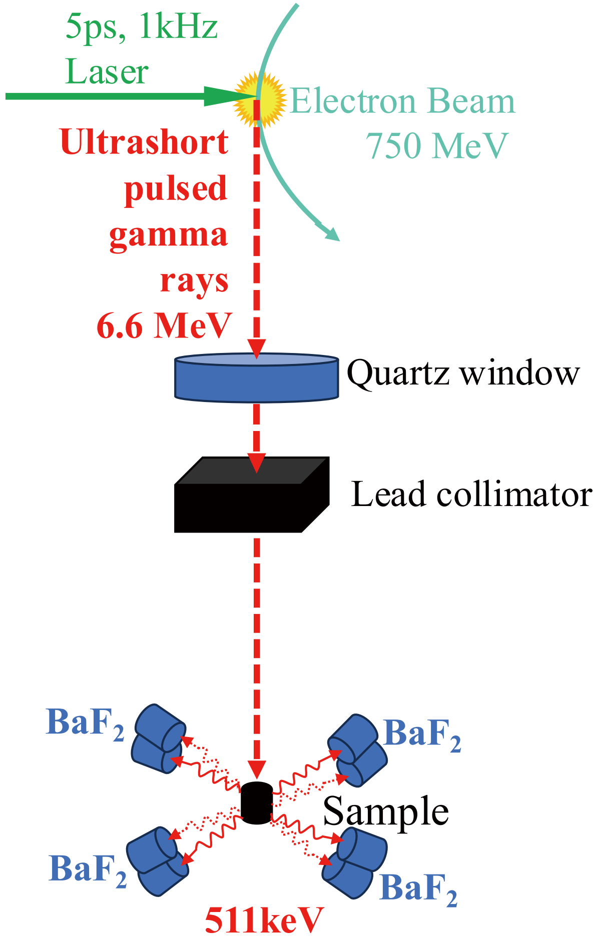


F.A. Selim. Positron annihilation spectroscopy of defects in nuclear and irradiated materials- a review. Materials Characterization 174 (2021) 110952

Experimental method



Different deformation to simulate progressive different stages of defect development



convolution integral: $$f(t) = \sum_{j=1}^{k_0} (a_j * R)(t) + B$$

where

$$a_j(t) = \begin{cases} A_j \exp(-(t - T_0)/\tau_j), & t > T_0 \\ 0, & t > T_0 \end{cases}$$

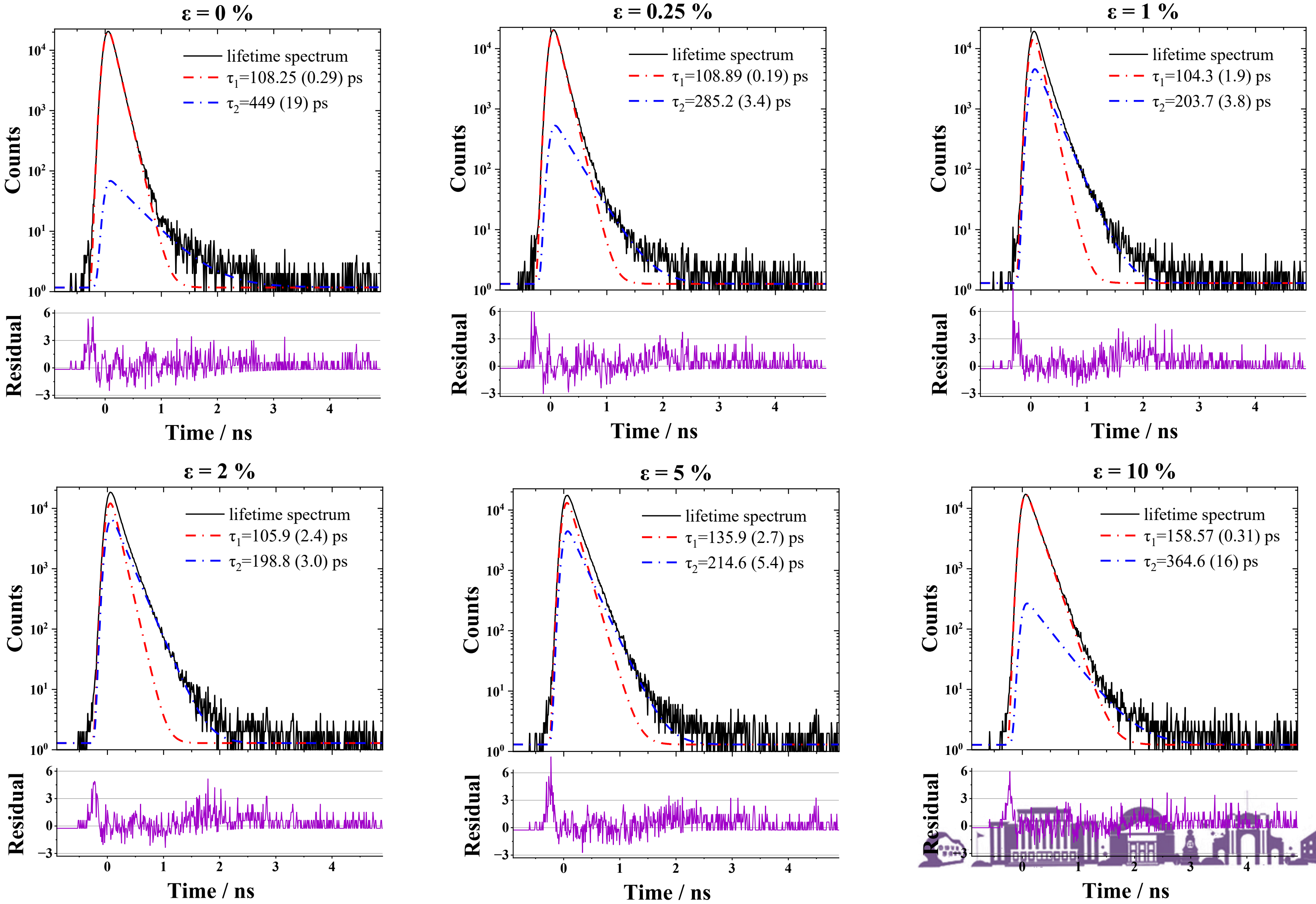
Positron lifetime component

$$R(t) = \sum_{p=1}^{k_g} w_p G_p(t) = \sum_{p=1}^{k_g} w_p \frac{1}{\sqrt{2\pi} s_p} \exp(-\frac{(t - \Delta_p)^2}{2 s_p^2})$$

time-resolution function

$$\sum_{p=1}^{k_g} w_p = 1 \qquad \int_{-\infty}^{\infty} R(t) dt = 1$$

Results

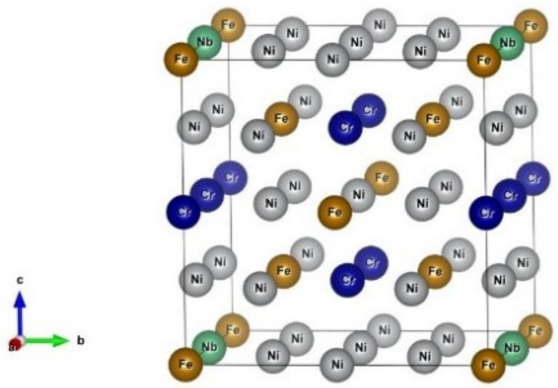

ε = 0 %
lifetime spectrum
τ1=108.25 (0.29) ps
τ2=449 (19) ps
ε = 0.25 %
lifetime spectrum
τ1=108.89 (0.19) ps
τ2=285.2 (3.4) ps
ε = 1 %
lifetime spectrum
τ1=104.3 (1.9) ps
τ2=203.7 (3.8) ps
ε = 2 %
lifetime spectrum
τ1=105.9 (2.4) ps
τ2=198.8 (3.0) ps
ε = 5 %
lifetime spectrum
τ1=135.9 (2.7) ps
τ2=214.6 (5.4) ps
ε = 10 %
lifetime spectrum
τ1=158.57 (0.31) ps
τ2=364.6 (16) ps
Counts
Residual
Time / ns

Results

Annihilation rate of e+-e- pairs using two component DFT method:

$$\frac{1}{\tau} = \lambda = \pi r_e^2 c \int n(r) n_+(r) \gamma(r) dr$$

Calculation of positron annihilation lifetime

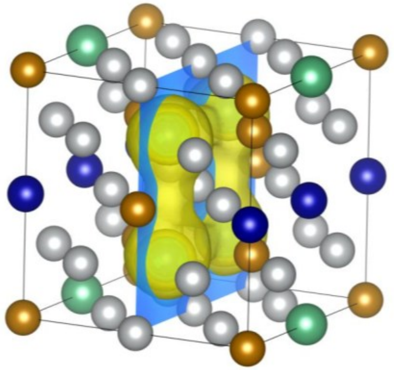


$Ni_{19}Fe_6Cr_6Nb$

a=b=c=7.1Å

Α=β=γ=90°

Prefect lattice



Vacancy-Ni

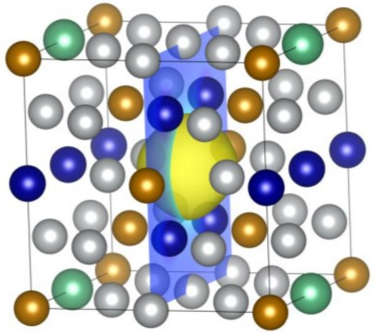
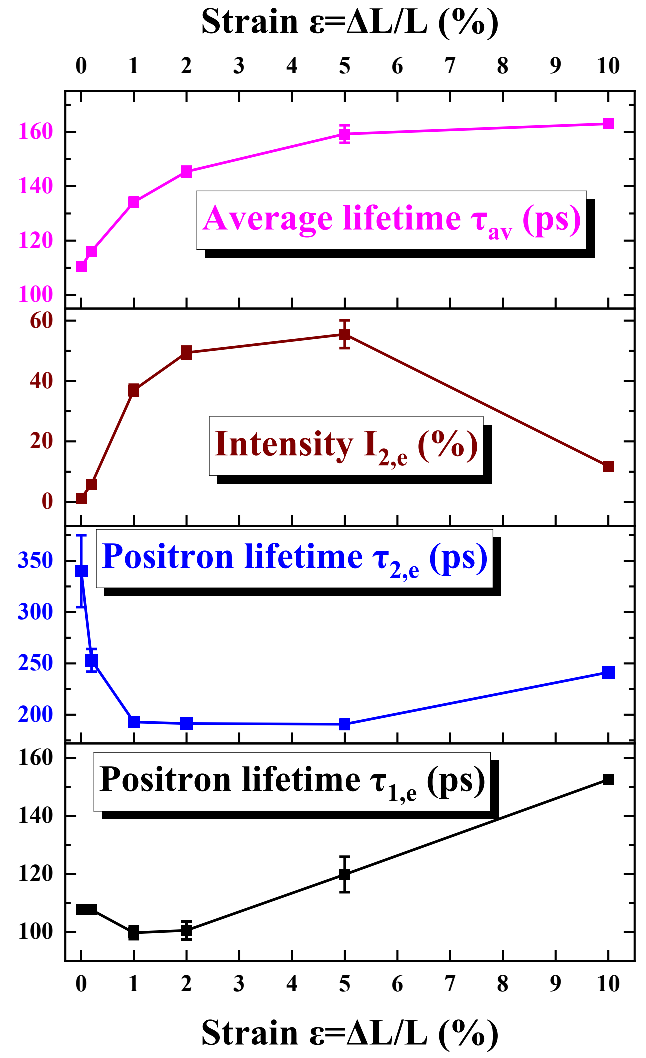


Table 1 Calculated positron state lifetimes (ps) for perfect lattice and defects in $Ni_{19}Fe_6Cr_6Nb$

Prefect lattice	Vacancy: Fe	Vacancy: Cr	Vacancy: Ni	Vacancy: Fe, Cr	Vacancy: Ni, Cr	Vacancy: Ni, Cr, Cr	Vacancy: Ni, Ni, Ni, Cr, Cr	Edge dislocation
105.7	160.5	184.1	164.0	178.4	181.1	190.3	224.5	145.5
Prefect	Vacancy							dislocation

Results

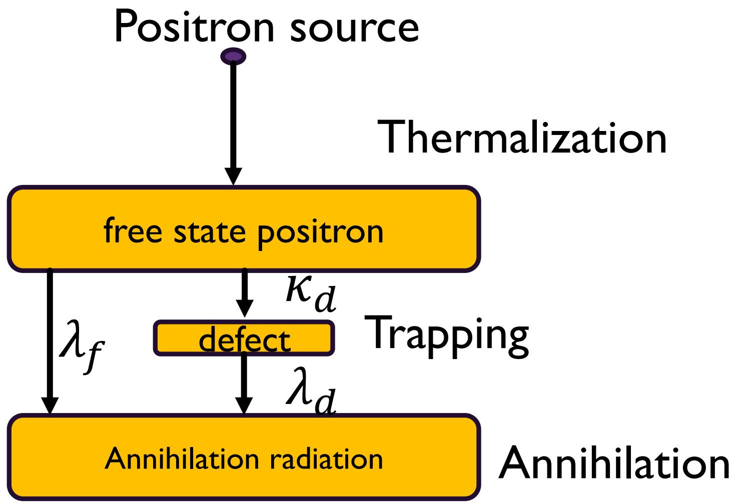


Trapping model

Assumption only one type defect in the sample：

$$\frac{dn_f(t)}{dt} = -\lambda_f n_f - \kappa_d n_f \quad (1)$$

$$\frac{dn_d(t)}{dt} = -\lambda_d n_d + \kappa_d n_f \quad (2)$$



n_f: the probability density of finding a delocalized (free) positron at the time t

n_d: the probability density of finding a localized positron at a defect at the time t

κ_d: the trapping rates to the defects in the system

λ_f: the free-positron annihilation rate

λ_d: the localized-positron annihilation rate.

The experimental spectrum can be described as:

$$S(t) = \lambda_f n_f + \lambda_d n_d = \left(\lambda_f - \frac{\lambda_d \kappa_d}{\lambda_f+\kappa_d-\lambda_d}\right) e^{-(\lambda_f+\kappa_d)t} + \frac{\lambda_d \kappa_d}{\lambda_f+\kappa_d-\lambda_d} e^{-\lambda_d t}$$

$$= \frac{I_1}{\tau_1} e^{-\frac{t}{\tau_1}} + \frac{I_2}{\tau_2} e^{-\frac{t}{\tau_2}}$$

$$\tau_1 = \frac{1}{\lambda_f+\kappa_d} \qquad I_1 = \frac{1}{\lambda_f+\kappa_d}\left(\lambda_f - \frac{\lambda_d \kappa_d}{\lambda_f+\kappa_d-\lambda_d}\right) = \frac{\lambda_f-\lambda_d}{\lambda_f+\kappa_d-\lambda_d}$$

$$\tau_2 = \frac{1}{\lambda_d} \qquad I_2 = \frac{\kappa_d}{\lambda_f+\kappa_d-\lambda_d}$$

CONCLUSIONS

- Two types of defects, dislocations and vacancies, can been identified with the aid of density functional theory.
- The observed increase in positron average lifetime with incremental tensile deformation can be used to characterized the defects in engineering materials for industrial use.
- Our work also provides valuable information on the defect formation of deformed samples contributing to a better understanding of fatigue damage.

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National Institutes of Natural Sciences
Institute for Molecular Science

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THANKS FOR YOUR ATTENTION!