SPATIAL CORRELATION OF OXIDE NANOPARTICLES AND DISPLACEMENT CASCADES INDUCED BY SWIFT HEAVY IONS IN ODS-ALLOYS

Alexei Prosvetov

Joint Institute for Nuclear Research, Dubna - Russia

Contact: alexei.v.prosvetov@gmail.com

Motivation

The most perspective materials for Gen-IV nuclear reactors are ODS-alloys.

ODS, Oxide Dispersion Strengthened, alloy is the metallic matrix based on iron or nickel with small (5-50 nm) oxide particles (Y_2O_3, Al_2O_3, Cr_2O_3, $Y_4Al_2O_9$).

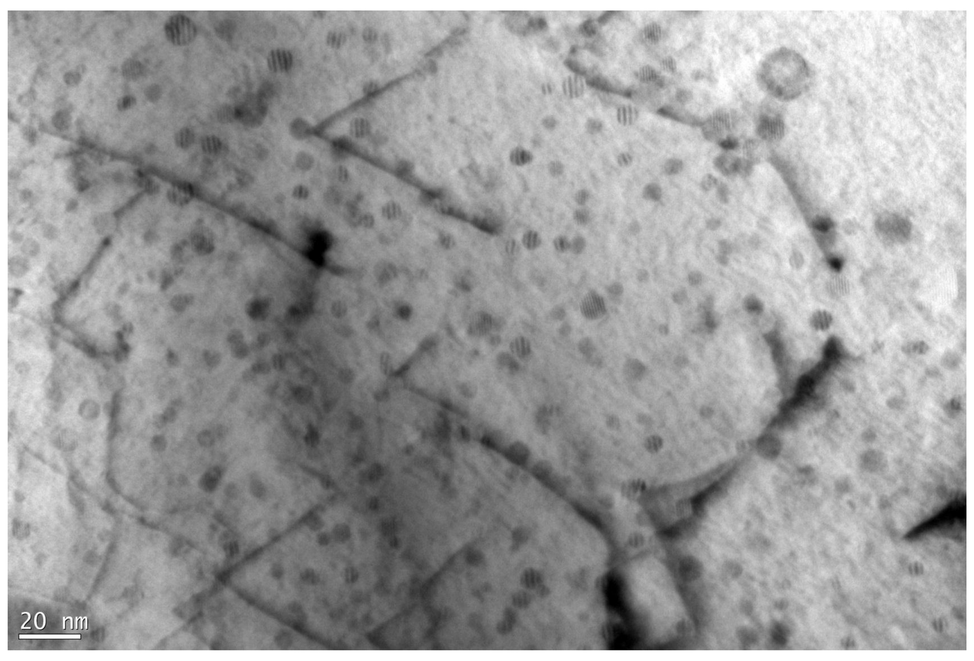
Radiation resistance of ODS-alloys depends on properties of oxide nanoparticles. Structural defects induced by swift heavy ion irradiation via electronic excitations and displacement cascades are concentrated in a small (5-10 nm) track region comparable with particle size. This can result in amorphization or dissolution of nano-oxides.

Aim of this work is to create a model, which

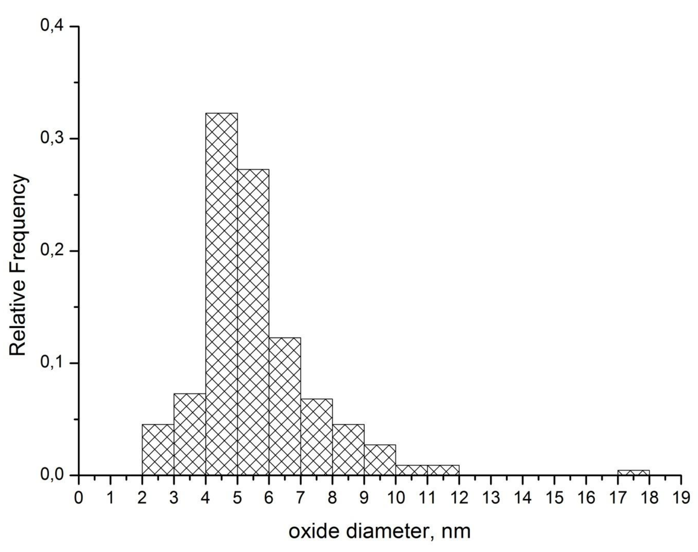
- ❑demonstrates spatial distributions of oxide nanoparticles and displacement cascades induced by heavy ions of fission fragment energy in ODS-alloy
- ❑estimates probability of overlapping of oxides and displacement cascades

Size distribution of oxide nanoparticles

The diameter of oxide particles was found using of TEM-images of ODS sample



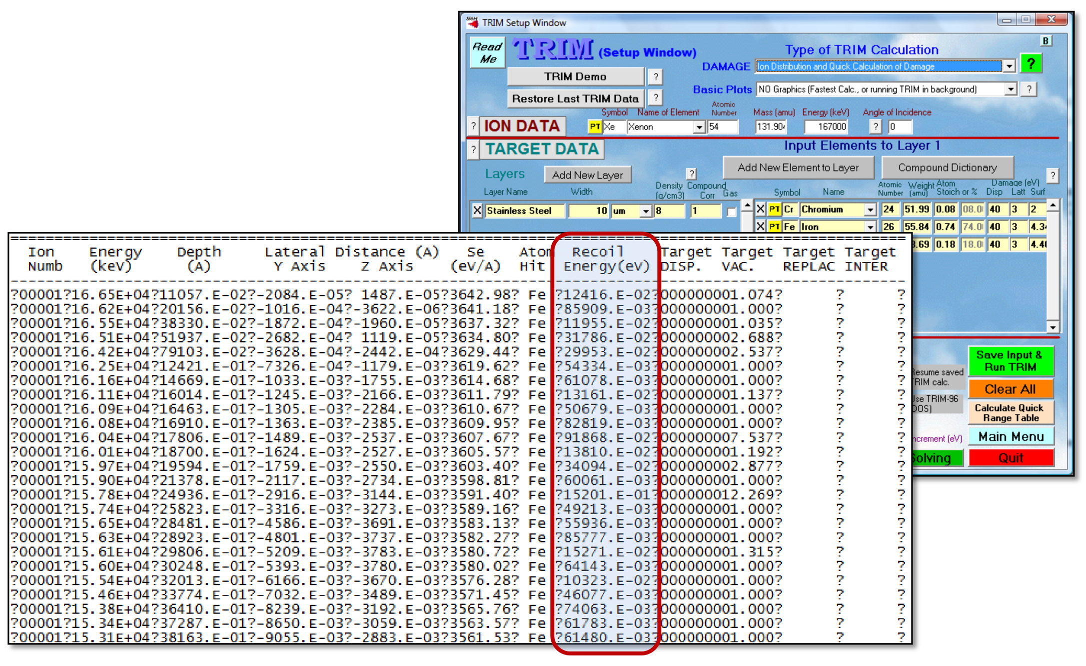
TEM-image of ODS-alloy Fe-15Cr-4Al-2W-0,35Y_2O_3 (KP4)
Centre for HRTEM, NMMU, Port Elizabeth, South Africa

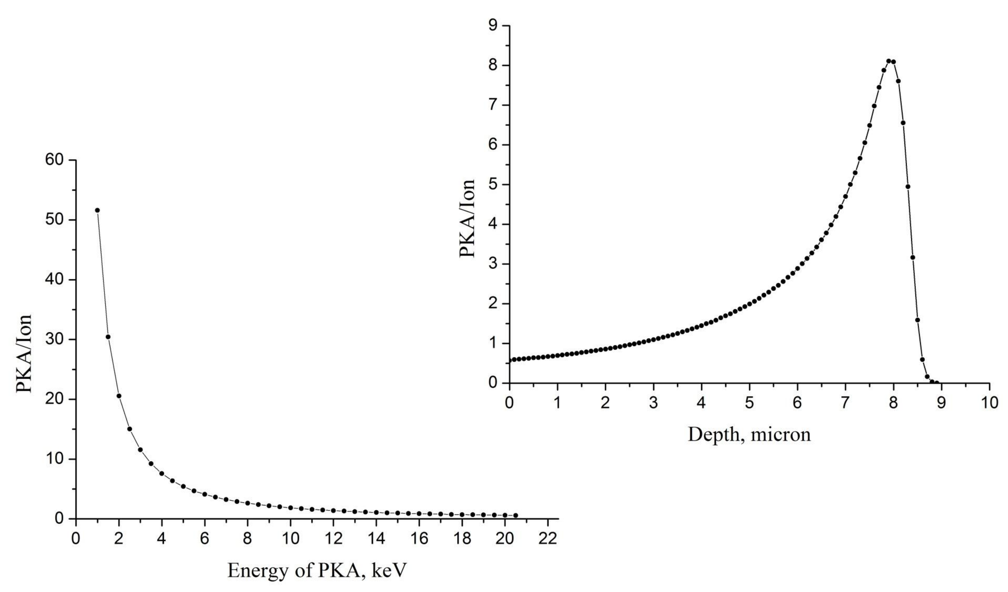


Size distribution of oxide particles in KP4 alloy

PKA spectrum

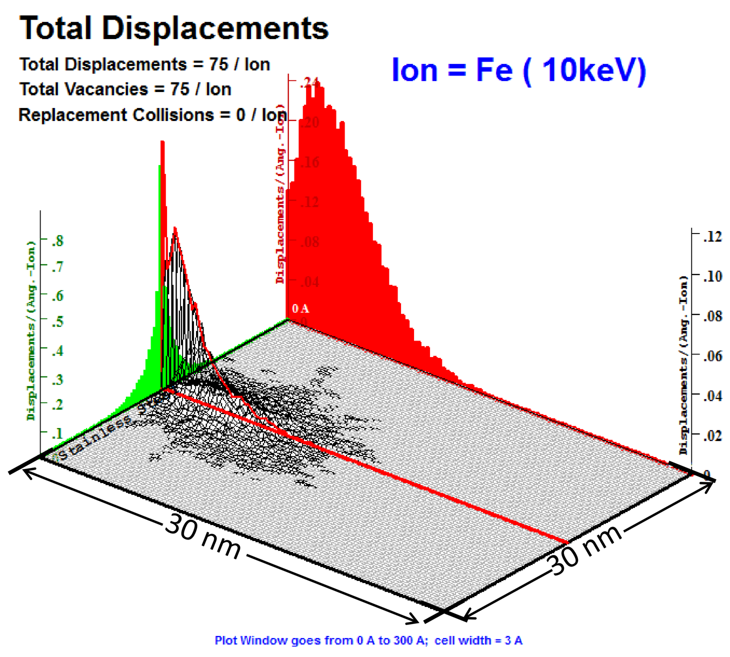
Primary knock-on atoms spectrum was found by using statistical data of SRIM-2011.





Primary knock-on atoms spectrum for 167 MeV Xe ions in KP4 alloy

Model of displacement cascade



Density of atomic displacements in cascade

Density of displacements in longitudinal direction:

$$f(x)_L = \frac{A_1}{\sigma \cdot \sqrt{\pi/2}} \cdot e^{-\frac{(x-x_c)^2}{2\sigma^2}}$$

Density of displacements in radial direction:

$$f(x)_R = \frac{2A_2}{\pi} \cdot \frac{\gamma}{4x^2 - \gamma^2}$$

Density functions depend on PKA energy as

$$C = a \cdot E^b,$$

C – parameter of density function ($A_1, x_c, \sigma, A_2, \gamma$),
E –PKA energy
a, b - adjustable parameters

The probability of overlapping of nanoparticles and cascades

We use geometric interpretation of probability, i.e. the ratio of the volumes.

Total volume of oxides particles:

$$V_{oxide} = \frac{4}{3}\pi \sum_i r_{oxide_i}^{\ 3}$$

Cascade volume:

$$V_{cascade} = \pi \cdot r_{cascade}^2 \cdot l_{cascade}$$

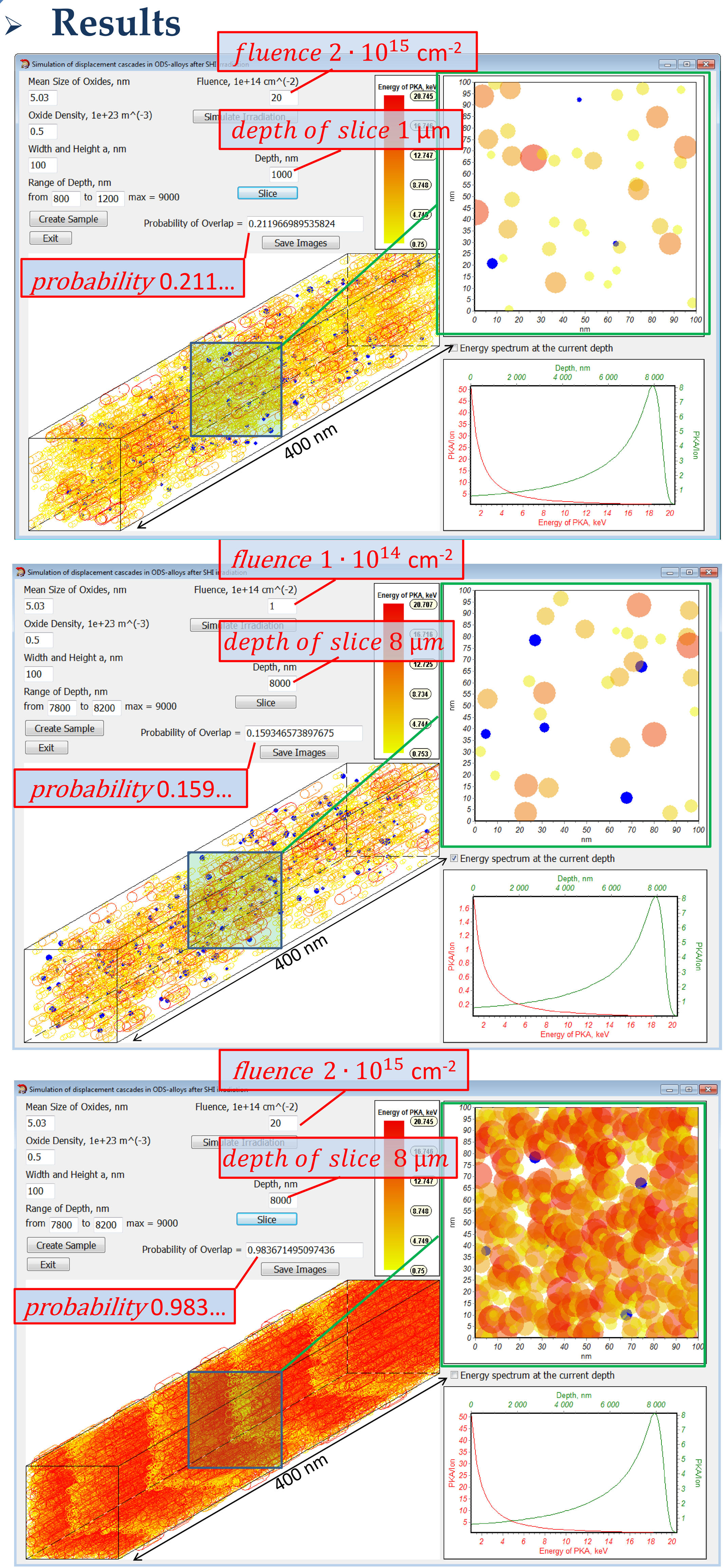
Probability of overlapping of cascade and oxide nanoparticle: $P = P_{cascade} \cdot P_{oxide}$

$$= \frac{V_{cascade}}{V_{bulk}} \cdot \left(1 - \frac{V_{cascade}}{V_{bulk} - V_{oxide}}\right)$$

For estimates of overlapping of different cascades we use the formula for the sum of the probability of joint events:

$$P(A+B) = P(A) + P(B) - P(AB)$$

Results



Model of the ODS sample irradiated by 1.2 MeV/amu Xe ions to fluences of $1{\cdot}10^{14}$ ·cm^{-2} and $2{\cdot}10^{15}$ ion·cm^{-2} in the subsurface layer and in the end-of-range region

Conclusions

- ✓Software tool was elaborated to demonstrate spatial distribution of oxide nanoparticles and displacement cascades induced by heavy ions of fission fragment energy in ODS-alloy
- ✓The probability of overlapping of nanosized oxides and displacement cascades is following:
  - 0.002 - Ion fluence $1{\cdot}10^{14}$ ion·cm^{-2} , depth 2 μm
  - 0.161 - Ion fluence $1{\cdot}10^{14}$ ion·cm^{-2}, end-of-range region (8 μm)
  - Probability is about 1
    - in the subsurface layer at a fluence of $5{\cdot}10^{16}$ ion·cm^{-2}
    - in the end–of-range region at a fluence $3{\cdot}10^{15}$ ion·cm^{-2}