Modeling of Radiation Effects and Microstructure Transformations in Construction Materials

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Dept. Modeling of Radiation Effects
and Microstructure Transformations in Construction Materials
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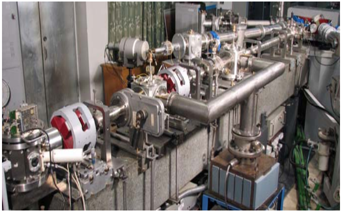
02/10/2014

GRID-cluster

Simulations & Validation

Scanning ion microprobe



RBS end-station

Scientific program: “Nuclear materials and reactor material science”

Facility development and study of point defects evolution and vacancy type clusters in construction materials under ion irradiation and hydrogen saturation

The main objectives are:

- to study statistical properties and distributions of defects and their complexes;
- to study the rearrangement of vacancy complexes

Theoretical approach

- *Ab initio*
- Molecular dynamics
- Kinetic Monte Carlo
- Rate theory

Validation of results ⟹

⟸ Parameters for calculation

Experimental approach

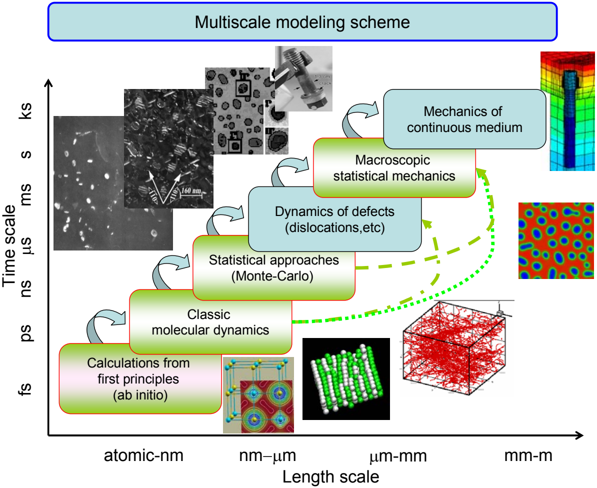
- Lifetime positron annihilation spectroscopy
- RBS/C and ERDA/C
- High dose implanter for metal ions
- XRD, microscopy etc

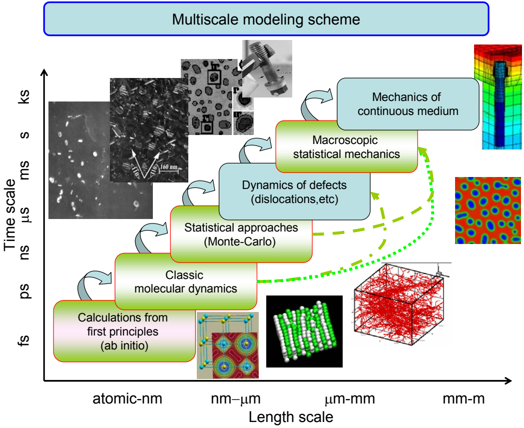
The main goals

- to develop theoretical models to study dynamics of point defects in construction materials (Zr, W, Ni, Be, etc.) under irradiation influence
- to study by numerical simulations rearrangement of point defect complexes in irradiated materials used in Next Generation Reactors.
- to determine and predict the behavior of structural materials under irradiation by the validation experiments

Dept. Modeling of radiation effects and microstructure transformations in construction materials

The research is focused on the study and characterization of radiation effects and microstructure transformations in condensed matter systems far from equilibrium.

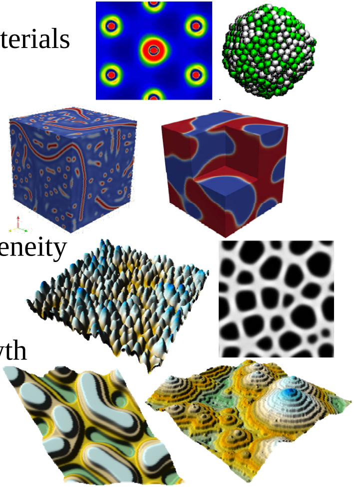




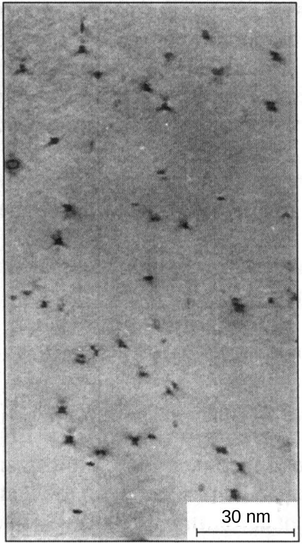
Within the framework of multi-scale modeling one can clarify the formation of defect structure, the redistribution of defects with the formation of clusters of point defects, the yield of defects to sinks, microstructure transformation induced by irradiation, the distribution of elastic stress fields at formation of clusters of defects and dislocations, changes in the morphology of the surface of irradiated materials in the process of sputtering.

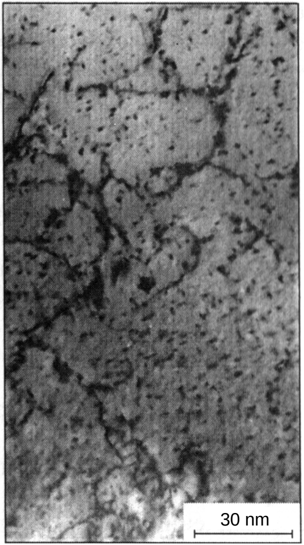
Research ineterests

- Ab-initio modeling of construction materials
- Molecular dynamics simulations
- Pattern formation of point defects
- Microstructure transformations
- Phase separation with elastic inhomogeneity
- Patterning at ion-beam sputtering
- Phase-field modeling of epitaxial growth
- Nano-islands formation at deposition



Typical defect structure in Ni irradiated by Ni^+ at $T = 300K$: 40dpa and 20dpa





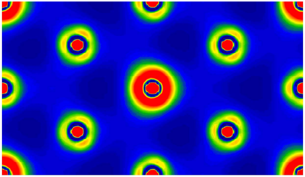
Modeling self-organization of vacancy clusters in irradiated materials

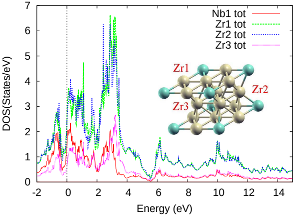
What has been done ?

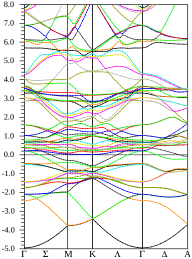
- Ab-initio modeling of $Zr - x\%Nb$ alloys with defects is performed: [$\mathbb{M}_3\mathbb{TREC}_\mathbb{S}$] — Metfiz. 2011; JNEP 2012, CMPH 2013
- Experimentally and theoretically (MD, KMC) evolution of defect structure is studied in annealed materials: [R.Stoller, K.Nordlund, et al.]
- Phase filed crystals method (PFC) is developed to study defects behavior in crystalline systems: [M.Grant, K.Elder, et al.]
- PFC is developed to study defect structure under irradiation conditions and at annealing the materials: [$\mathbb{M}_3\mathbb{TREC}_\mathbb{S}$] — Physica A 2010; CEJP 2011; UJP 2012; UFM 2012
- Rate theory for describing defects dynamics is proposed: [C.Abromeit, G.Marten, F.Kh.Mirzoev, et al.]
- Rate theory is developed to study self-organization of point defects in materials under irradiation: [$\mathbb{M}_3\mathbb{TREC}_\mathbb{S}$] — EPJB 2012; UJP 2013; REDS 2013; PRE 2014

Ab-initio modeling

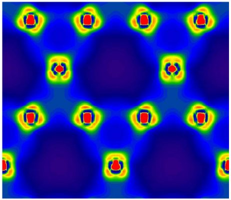
Alloys Zr – Nb

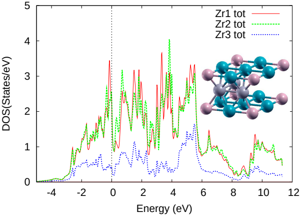


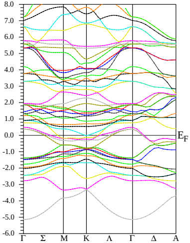




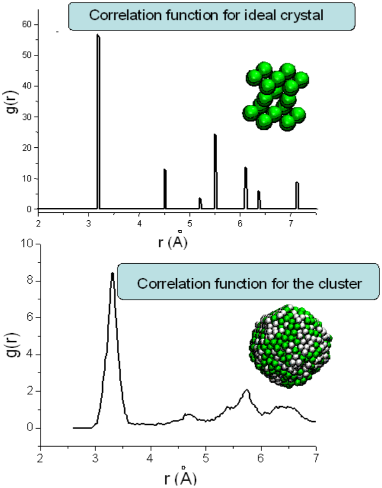
Zr+vacancies







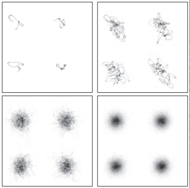
Molecular Dynamics simulations

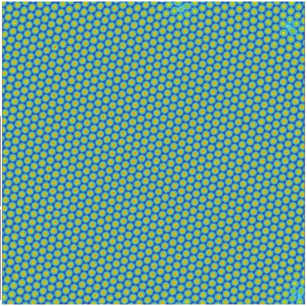


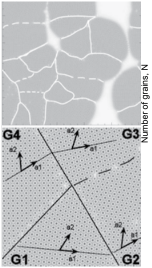
Vacancies

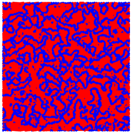
Phase field crystals method

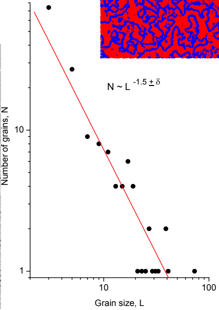
Atomic density field:



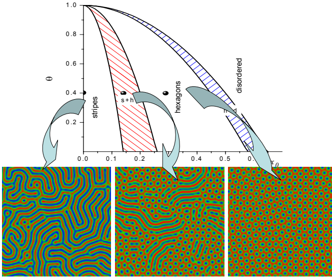






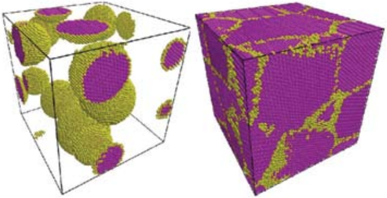


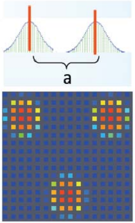
Crystalline system subjected to irradiation (PFC)

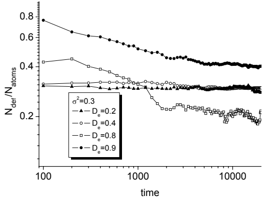


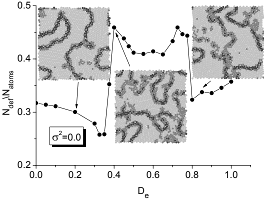
Irradiation: Exp 1 Irradiation: Exp 2

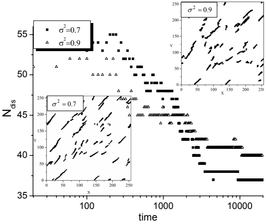
Microstructure before and after irradiation (PFC)



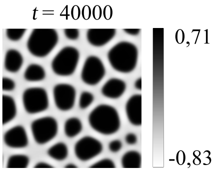




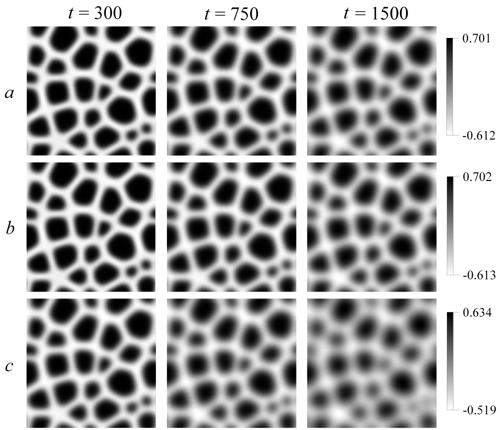




Phase separation of binary allays with elastic inhomogeneity



Coherent configuration of the binary alloy



Evolution of composition difference at different irradiation conditions

Modeling of defect structure evolution in systems subjected to irradiation (Rate theory)

Two-component model of point defects dynamics

$$\begin{aligned} \partial_t c_v &= K - D_v S_v (c_v - c_v^0) - \alpha c_v c_i; \\ \partial_t c_i &= K - D_i S_i c_i - \alpha c_v c_i. \end{aligned} \tag{1}$$

Sinks densities:

$$S_{v,i} = Z_{\{v,i\}N} \rho_N (1 + \rho_v^* + \rho_i^*), \quad \rho_{v,i}^* \equiv \rho_{v,i}/\rho_N, \quad \mu \equiv (1 + \rho_v^* + \rho_i^*) \tag{2}$$

Adiabatic elimination procedure: $D_v/D_i \equiv \delta \ll 1$

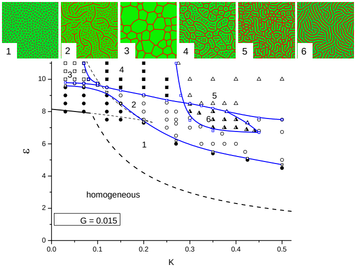
$$\partial_t x = K - \mu(x - x_0) - \frac{Kx}{\frac{\mu(1+B)}{\delta} + x} + G e^{\varepsilon x/(1+x^2)}, \quad \varepsilon = \frac{E}{k_B T} \tag{3}$$

Self-Organization of Vacancy Clusters (2D-modeling)

Evolution of vacancy concentration field

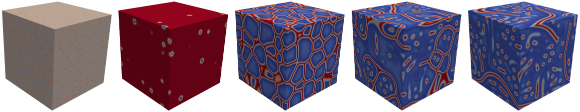
$$\partial_t x = K - \gamma x + G\exp(\varepsilon x/(1+x^2)) - \nabla\cdot\vec{J}; \qquad (4)$$
$$\vec{J} = -D[\nabla x - \varepsilon x \nabla(x + r_0^2\nabla^2 x)].$$

1 2 3 4 5 6



[Eur.Phys.Jour.B, v.85, 383, (2012)]

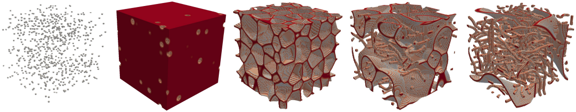
Self-Organization of Vacancy Clusters (3D-modeling)



Total concentration Cross-section

[Cond.Mat.Phys., v.16, 33001, (2013)]

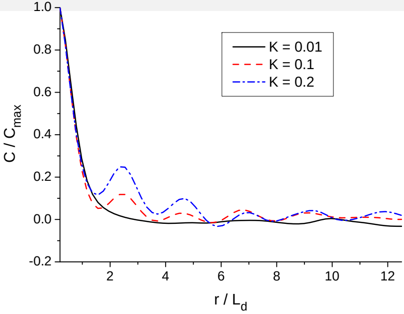
Self-Organization of Vacancy Clusters (3D-modeling)

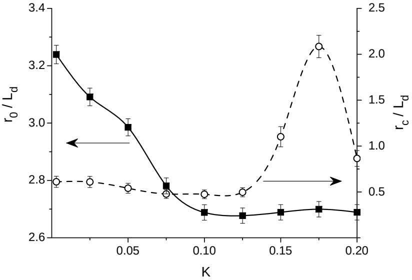


Clusters of defects

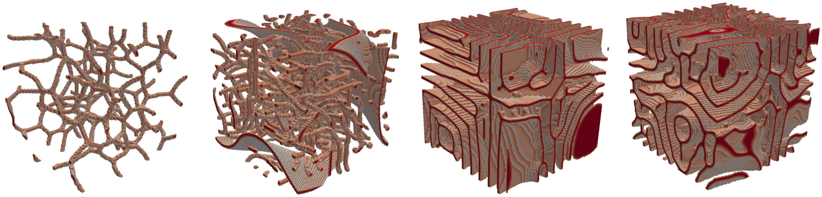
[Cond.Mat.Phys., v.16, 33001, (2013)]

Correlation analysis





K=0.025 K=0.075 K=0.175 K=0.2



[Cond.Mat.Phys., v.16, 33001, (2013)]

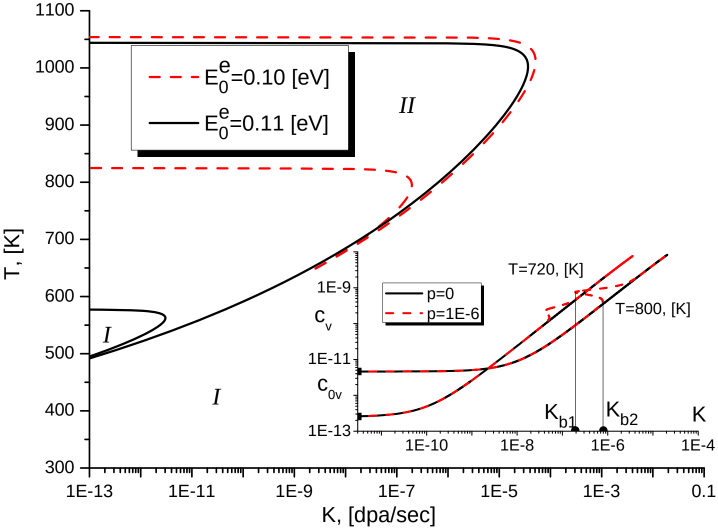
Vacancy Clusters in Ni under Irradiation

Evolution equation for the loop densities:

$$\begin{aligned} \partial_t \rho_i &= \frac{2\pi N}{b}\left(\varepsilon_i K + D_i Z_{iI} c_i - D_v Z_{vI}(c_v - c_{v0})\right); \\ \partial_t \rho_v &= \frac{1}{b r_v^0}\left(\varepsilon_v K - \rho_v [D_i Z_{iV} c_i - D_v Z_{vV}(c_v - c_{v0})]\right). \end{aligned} \tag{5}$$

Vacancy formation energy	E_v^f	1.8	eV
Vacancy migration energy	E_v^m	1.04	eV
Interstitial migration energy	E_i^m	0.3	eV
Elastic interaction energy	E_0^e	$0.01 \div 0.2$	eV
Vacancy Diffusion coef.	D_v	$6 \cdot 10^{-5} e^{-E_v^m/T}$	m^2/s
Interstitial Diffusion coef.	D_i	$10^{-7} e^{-E_i^m/T}$	m^2/s
Equil. vacancy conc.	c_{0v}	$e^{-E_v^f/T}$	—
Debye frequency	ω_D	$1.11 \cdot 10^{13}$	s^{-1}
Vacancy loop radius	r_0	$1.5 \cdot 10^{-9}$	m
Cascade collapse efficiency	ε_v, ε_i	0.1, 0.01	—
Dislocation density	ρ_N	$10^{12} \div 10^{15}$	m^{-2}
Atomic volume	Ω	$1.206 \cdot 10^{-29}$	m^3

Vacancy Clusters in Ni under Irradiation



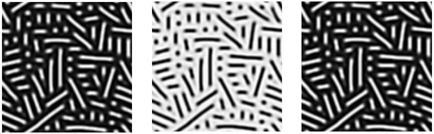
[Rad.Eff.Def.Solids, v.169, 418, (2014)]

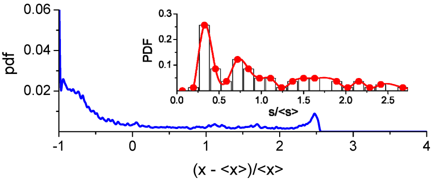
Vacancy Clusters in Ni under Irradiation

Reactor conditions

$$T = 773\text{K},\ K = 10^{-6}\text{dpa/sec}$$

x ρ_i ρ_v





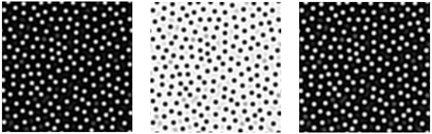
Linear size of vacancy clusters:

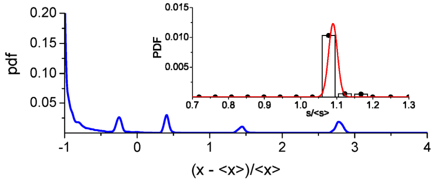
$\langle d_0 \rangle \sim 6$ nm

Accelerator conditions

$$T = 900\text{K},\ K = 10^{-3}\text{dpa/sec}$$

x ρ_i ρ_v





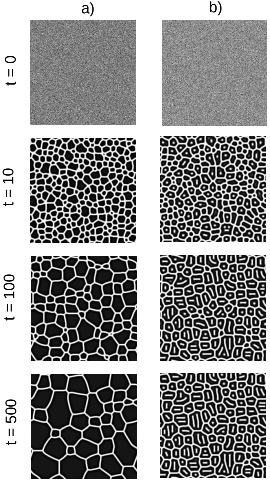
Linear size of vacancy clusters:

$\langle d_0 \rangle \sim 7.5$ nm

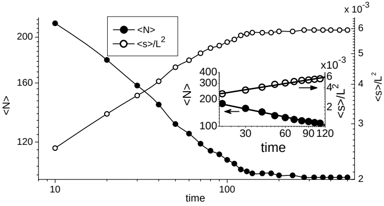
[Rad.Eff.Def.Solids, v.169, 418, (2014)]

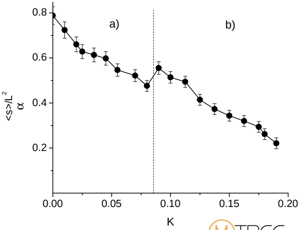
Delayed grain growth

Scaling properties $\langle s(t)\rangle \propto t^{\alpha}, \quad \langle N(t)\rangle \propto t^{-\alpha}$



$\varepsilon = 10,\ K = 0.05$ $\qquad$ $\varepsilon = 10,\ K = 0.15$

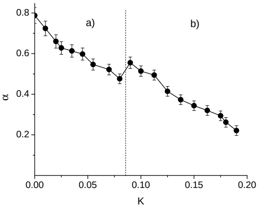


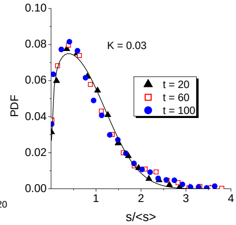


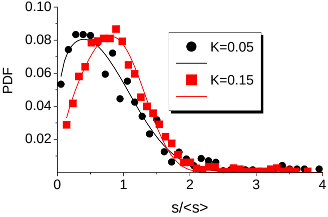
[Phys.Rev.E, v.89, 042133, (2014)]

Distributions over grains area

Scaling properties $\langle s(t)\rangle \propto t^{\alpha}, \quad \langle N(t)\rangle \propto t^{-\alpha}$







$$\mathrm{PDF}\left(\frac{s}{\langle s\rangle}, t\right) = N_0 t^{-\frac{2}{1-\varkappa}} \left(\frac{s}{\langle s\rangle}\right)^{-(1+\varkappa)/2}$$

$$\exp\left(-\frac{1}{\sigma^2}\left[\frac{\lambda+\chi}{D(2-\varkappa)}\left(\frac{s}{\langle s\rangle}\right)^{1-\varkappa/2} + \sqrt{\frac{s}{\langle s\rangle} - \frac{1}{2}\frac{s}{\langle s\rangle}}\right]\right), \quad \varkappa = 1 - \frac{2}{\alpha(K)}$$

[Phys.Rev.E, v.89, 042133, (2014)]

Main conclusions

1. We have studied the dynamics of point defects and rearrangement of vacancy complexes in materials under irradiation in the framework of multi-scale modeling scheme.
2. Obtained results of numerical simulations can be validated by experimental investigations on accelerator facilities of IAP NAS of Ukraine.
3. Obtained results can be used to predict and describe processes of defect structure formation, redistribution of defects with the formation of clusters of point defects, yield of defects to sinks and microstructure transformation induced by irradiation for construction materials of the Next Generation Reactors

Perspectives of Simulation-Validation program

1. Studying energetic characteristics of vacancy ensemble in W and Be by modeling from first principles and molecular dynamics. Validation of theoretical results by treatment results in exposure of Fe, Ni, W and Be by beams of Fe^+, Be^+, He^+ and H^+.

2. Measurement of the location of the interstitial atoms and defects in materials based on Fe and Ni, W and Be. Investigation of segregation of impurities at the grain boundaries of structural steels.

3. Modeling formation of vacancy clusters and superlattices of vacancies in Fe, Ni, W and Be within the framework of phase field approach and rate theory. Validation of the model parameters of vacancy ensembles by measurement of vacancy-type defects concentration by positron annihilation. Measurement of profiles of interstitials by PIXE, PIGE, RBS, ERDA.

4. Modeling surface erosion during sputtering and studying surface morphology transformations of Fe and Ni, W and Be based materials, bombarded by beams of H^+, He^+, Fe^+, Ni^+, W^+ and Be^+.

ThanX for attention

Special thanX:

Prof. D.Kharchenko
Dr. S.Kokhan
Dr. I.Lysenko
Dr. O.Schekotova

Organizers
for invitation & financial support

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Dr. O.Schekotova M3TRECs

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Welkome to Sumy