Modeling plastic deformation and mechanical properties change of Zr-Sn alloys subjected to irradiation in three dimensions

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Abstract

In order to predict the durability and reliability of construction materials, which are subjected to irradiation and mechanical loads, it is necessary to investigate an irradiation influence on a change in their mechanical properties. In this work we consider binary Zr-Sn alloy and perform mechanical testing in the form of shear deformation with a constant strain rate to study mechanical properties change of alloy under irradiation. Based on the phase field approach including elastic contribution in the framework of the nonlinear elasticity [1, 2] we perform the three-dimensional numerical modeling of plastic flow in the previously prepared Zr-Sn alloy samples before and after irradiation. Simulations in 3D allow to get detailed information about rearrangement of elastic fields and defect structure development in a bulk.

Introduction

Main tasks are:

1. To study evolution of slip planes and dislocation loops in the bulk of Zr-Sn alloy sample under applied shear strain.
2. To build the stress-strain curves at different irradiation regimes (irradiation temperature, dose rate) and strain rates.
3. To explore a change in mechanical properties of Zr-Sn alloy at different irradiation conditions and analyze the influence of strain rate on plasticity and strength.
4. To investigate the dependencies of the strain hardening coefficient and elastic energy on the strain at different irradiation parameters.

The Model

We consider binary Zr-Sn alloy with atoms of two sorts and vacancies.

Gibbs free energy

$$\mathcal{G} = \int_V \left[V_m^{-1} G(c, c_v) + \frac{\epsilon_c^2}{2}(\nabla c)^2 + \frac{\epsilon_v^2}{2}(\nabla c_v)^2 + G_{el}(\mathbf{u}, c, c_v) \right] \mathrm{d}\mathbf{r} \qquad (1)$$

c – composition field ($c \equiv c_{Zr}$), c_v – concentration of vacancies
$\boldsymbol{u} = (u_x, u_y, u_z)$ – elastic displacement vector

$$G_{el}(\mathbf{u}, c, c_v) = \alpha e_1 c + \beta e_1 c_v + g_{el}(\mathbf{u}, c) \qquad (2)$$

Elastic energy density

$$g_{el}(\mathbf{u}, c) = \frac{1}{2} K e_1^2 + \Phi(c, e_2, e_3) + \Psi(c, e_4, e_5, e_6) \qquad (3)$$

Elastic energy of tensile and compressive deformation

$$\Phi(c, e_2, e_3) = \frac{\mu}{8\pi^2}\left[3 - \cos(2\pi e_+) - \cos(2\pi e_-) - \cos\left(\frac{4\pi e_3}{\sqrt{3}}\right)\right] \qquad (4)$$

Elastic energy of shear deformation

$$\Psi(c, e_4, e_5, e_6) = \frac{\mu}{4\pi^2}\left[3 - \cos(2\pi e_4) - \cos(2\pi e_5) - \cos(2\pi e_6)\right] \qquad (5)$$

Elastic strain components
(e_1 – dilation strain, e_2, e_3 – tetragonal strains,
e_4, e_5, e_6 – shear strains):

$$\begin{array}{l} e_1 = \partial_x u_x + \partial_y u_y + \partial_z u_z, \quad e_\pm \equiv e_2 \pm e_3/\sqrt{3} \\ e_2 = \partial_x u_x - \partial_y u_y, \quad e_3 = (2\partial_z u_z - \partial_x u_x - \partial_y u_y)/\sqrt{3} \\ e_4 = \partial_x u_y + \partial_y u_x, \quad e_5 = \partial_y u_z + \partial_z u_y, \quad e_6 = \partial_z u_x + \partial_x u_z \end{array} \qquad (6)$$

Elastic moduli:

$$\begin{array}{ll} K = K^\alpha c + K^\beta (1 - c) & \text{– bulk elastic modulus} \\ K^\alpha, K^\beta & \text{– bulk moduli of Zirconium and Tin} \\ \mu = \mu^\alpha c + \mu^\beta (1 - c) & \text{– shear modulus} \\ \mu^\alpha, \mu^\beta & \text{– shear moduli of Zirconium and Tin} \end{array} \qquad (7)$$

The Model

Dynamics of the composition and vacancy concentration fields is given by the diffusive equations:

$$\partial_t c = -\nabla \cdot \mathbf{J}_c, \quad \mathbf{J}_c = -L_c \nabla \frac{\delta \mathcal{G}}{\delta c} + \xi_c(\mathbf{r}, t) \qquad (8)$$

$$\partial_t c_v = -\nabla \cdot \mathbf{J}_v, \quad \mathbf{J}_v = -L_v \nabla \frac{\delta \mathcal{G}}{\delta c_v} + \xi_v(\mathbf{r}, t) \qquad (9)$$

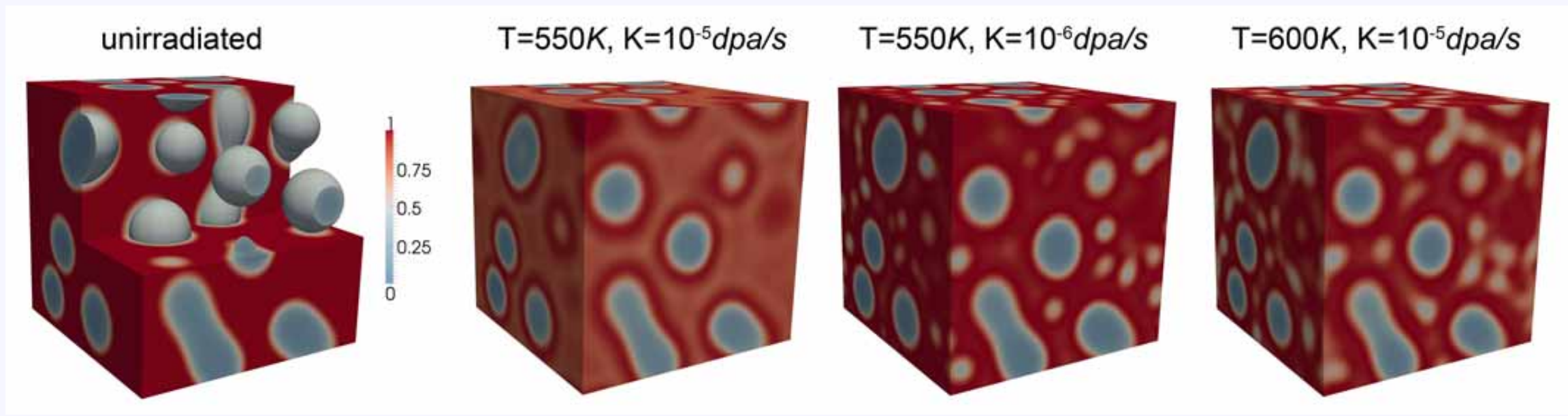
$\mathbf{J}_c$, $\mathbf{J}_v$ – diffusion fluxes, L_c, L_v – kinetic coefficients
Dynamics of the elastic fields

$$\rho \frac{\partial \boldsymbol{v}}{\partial t} = \eta_0 \nabla^2 \boldsymbol{v} + \nabla \cdot \overset{\leftrightarrow}{\sigma} \qquad (10)$$

$\boldsymbol{v} = \partial \boldsymbol{u}/\partial t$ – lattice velocity, ρ – mass density, η_0 – shear viscosity, $\overset{\leftrightarrow}{\sigma} = \{\sigma_{ij}\}$ – elastic stress tensor ($\nabla \cdot \overset{\leftrightarrow}{\sigma} = -\delta\mathcal{G}/\delta\boldsymbol{u}$)

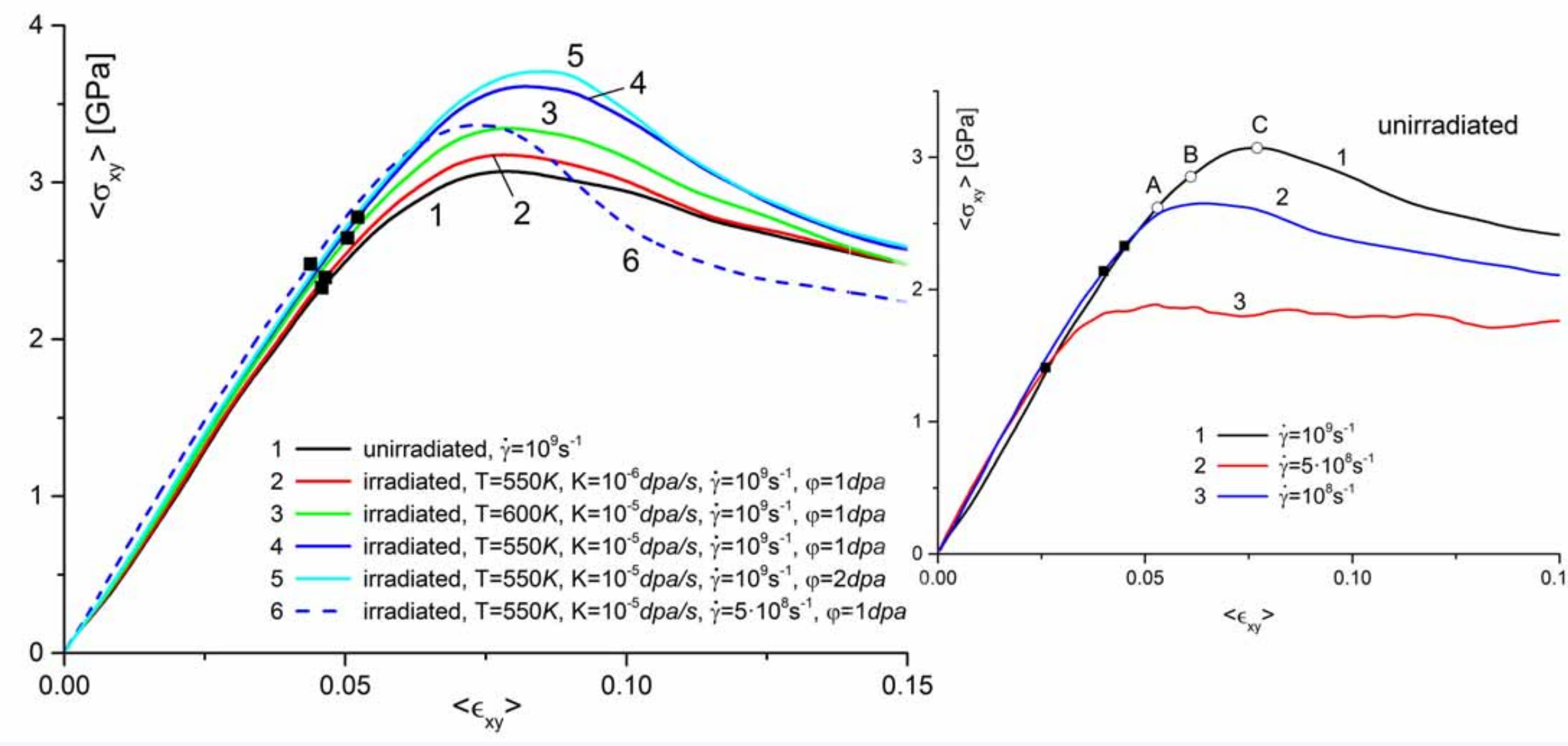
Simulations

Configurations of binary Zr-10%Sn alloy before and after irradiation (1 dpa)



Shear deformation $\gamma = \dot{\gamma} t$ with constant strain rate $\dot{\gamma}$

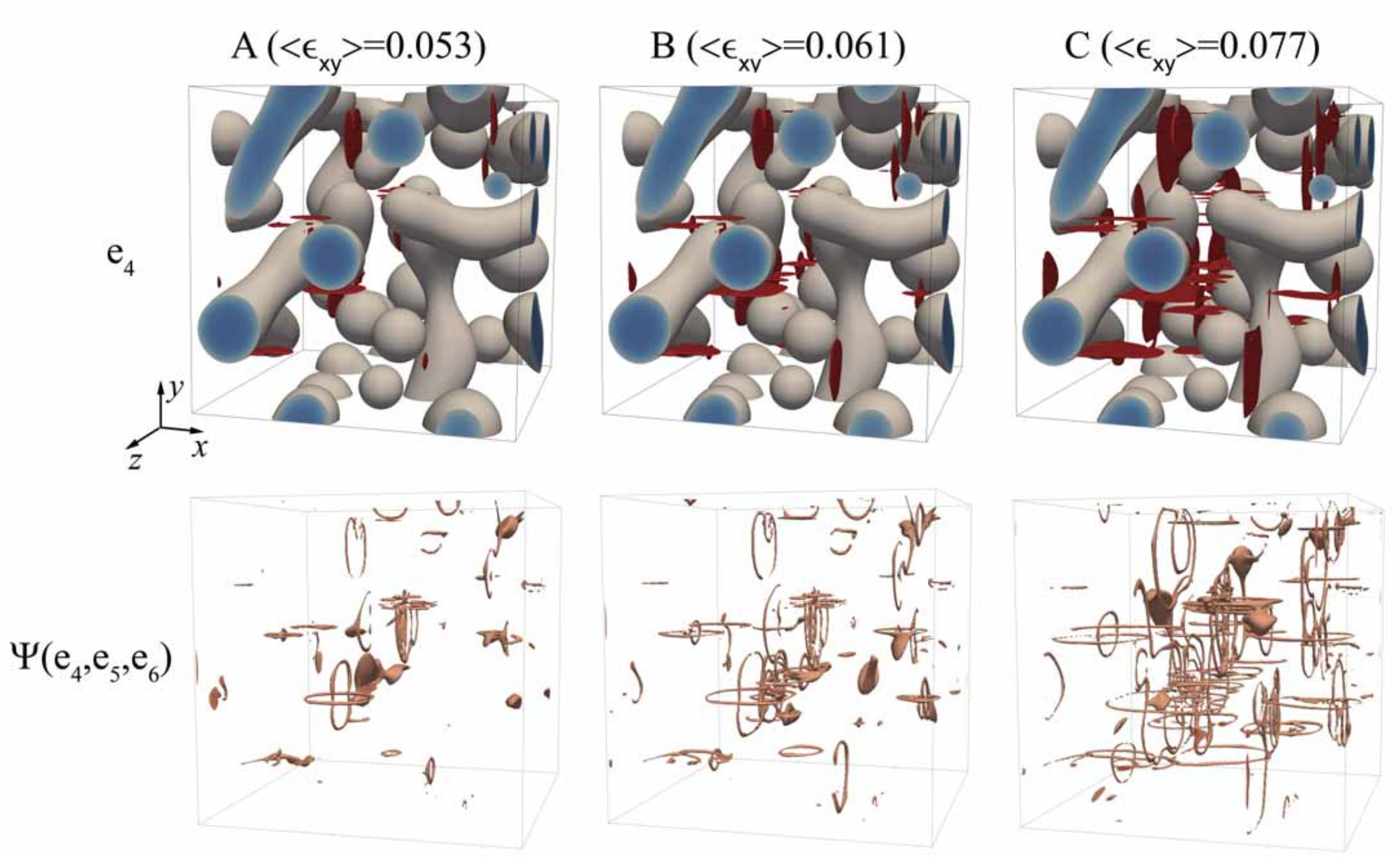
Stress-strain curves



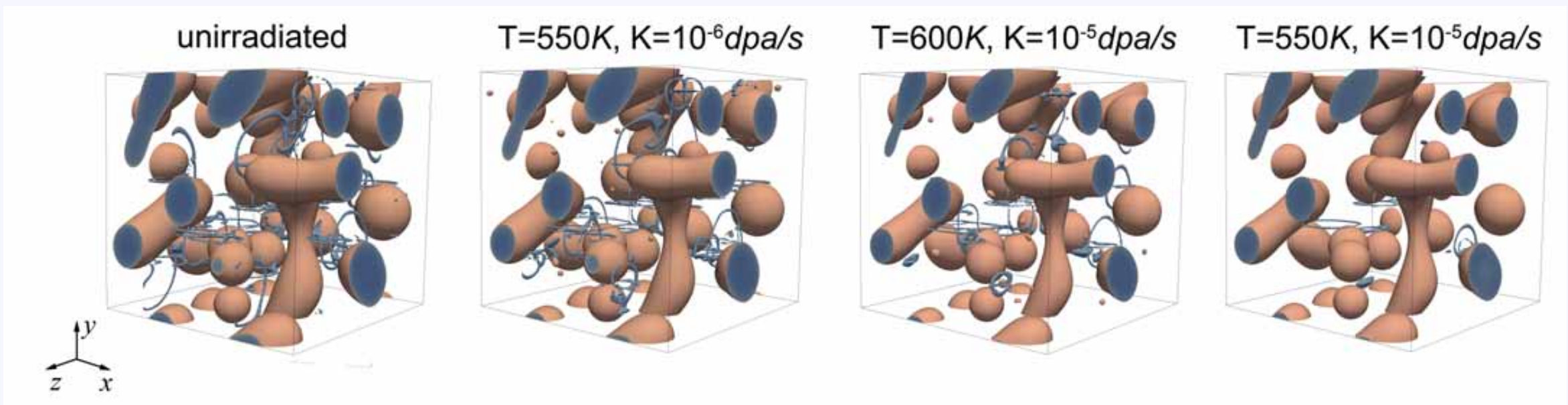
Values of yield strength σ_y and ultimate strength σ_u

temperature T, K	unirradiated			600	550	550		
dose rate $\mathcal{K}$, dpa/s				10^{-5}	10^{-6}	10^{-5}		
strain rate $\dot{\gamma}$, s^{-1}	10^8	$5 \cdot 10^8$	10^9	10^9	10^9	10^8	$5 \cdot 10^8$	10^9
σ_y, GPa	1.41	2.14	2.33	2.64	2.39	2.19	2.48	2.78
σ_u, GPa	1.89	2.65	3.07	3.34	3.17	2.66	3.36	3.61

Elastic fields evolution (slip planes and dislocation structure) for unirradiated alloy under shear ($e_4 > 0.6$ (red), $\Psi > 0.22$)

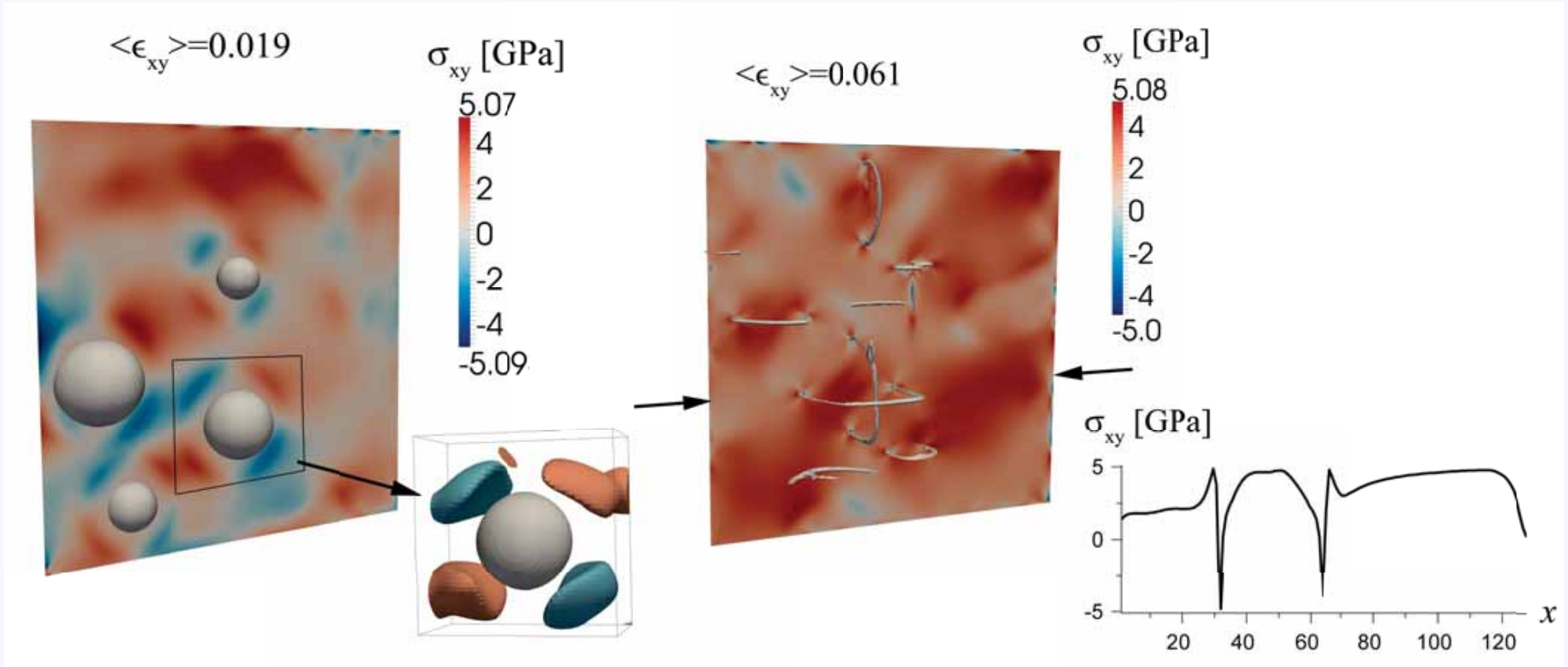


Irradiation influence on elastic fields ($\Psi > 0.22$, $\langle \epsilon_{xy} \rangle = 0.077$)

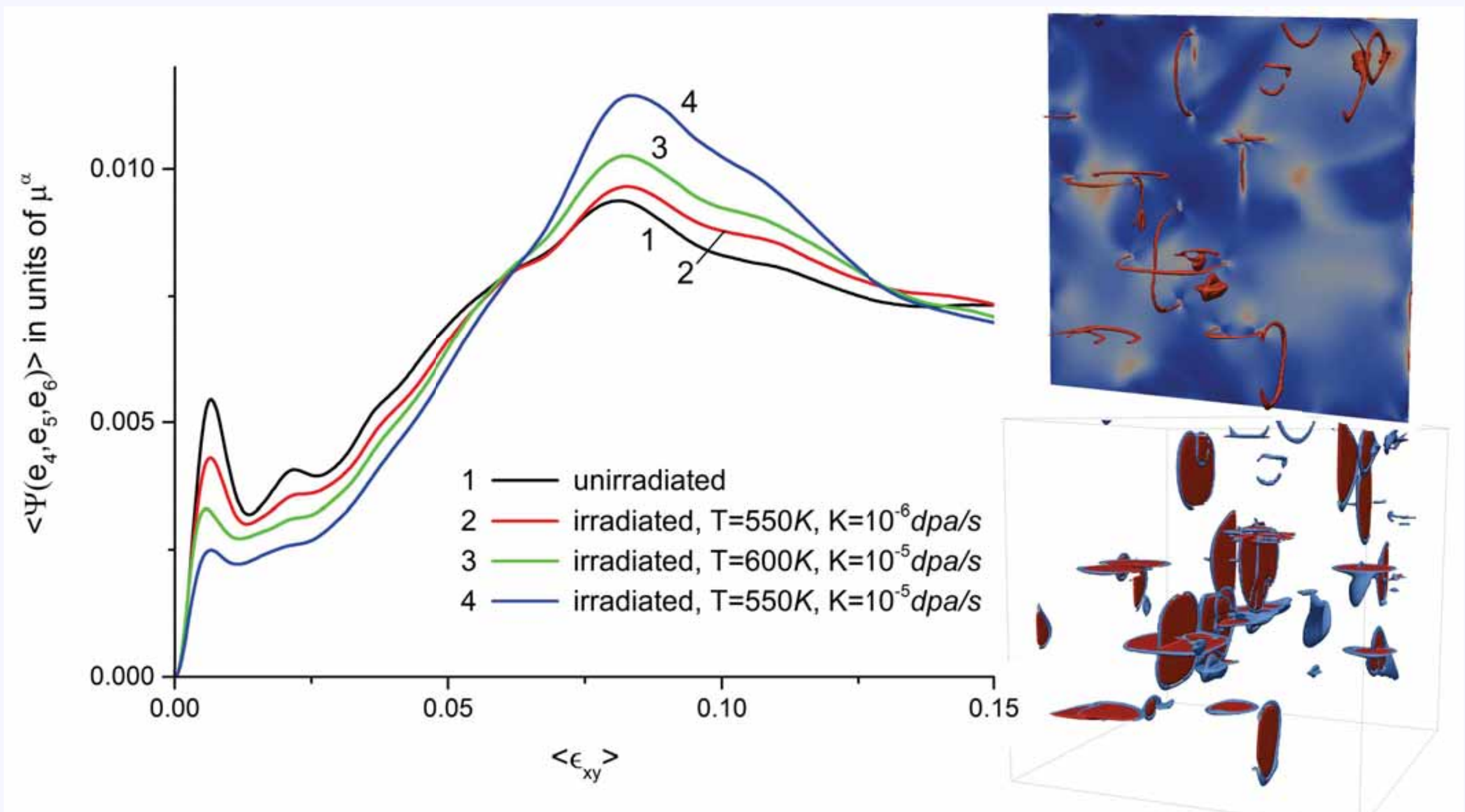


Simulations

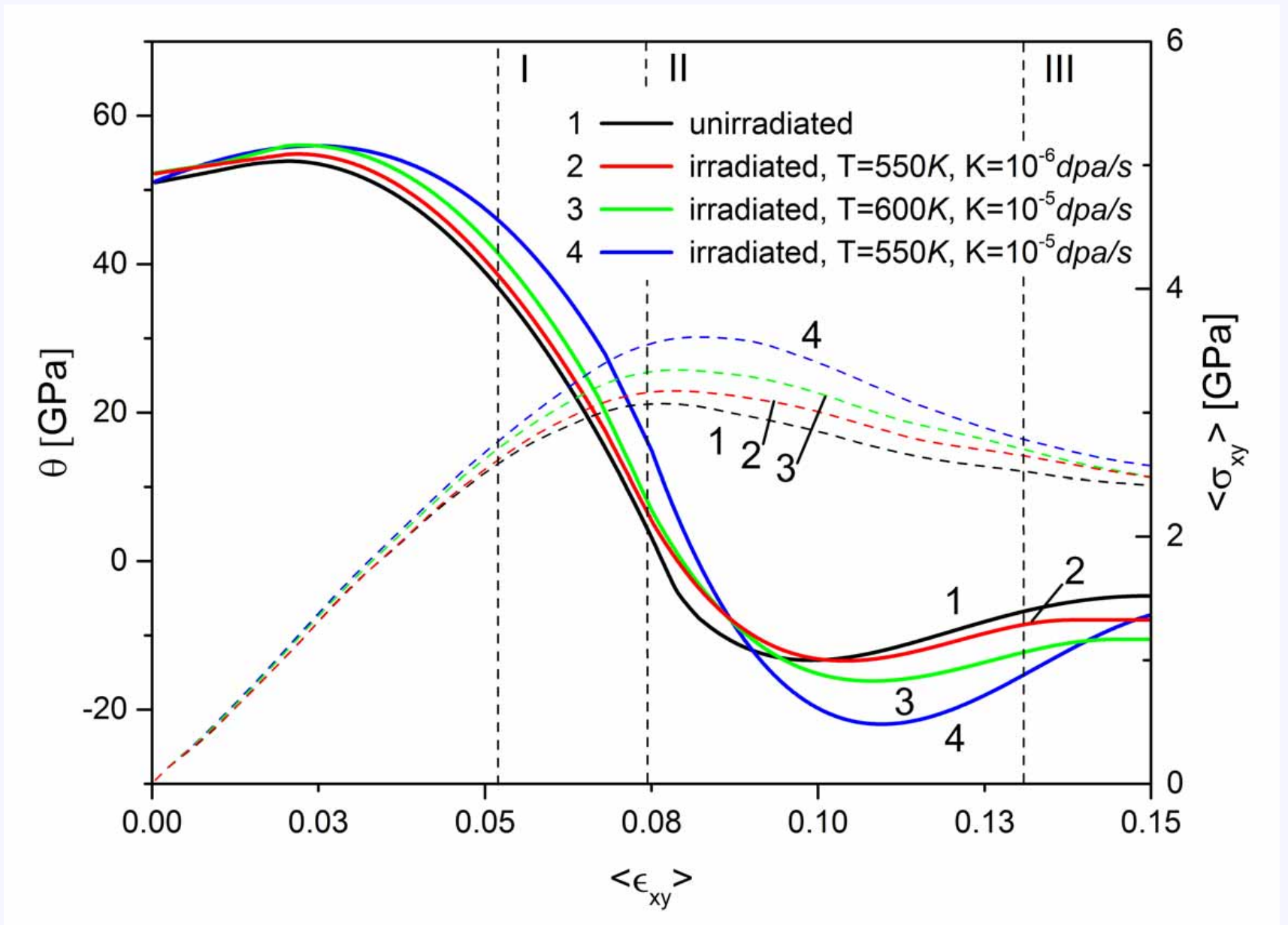
Distribution of shear stresses for unirradiated alloy



Elastic energy



Dependencies of strain hardening coefficient $\theta = \partial \langle \sigma_{xy} \rangle / \partial \langle \epsilon_{xy} \rangle$ on deformation $\langle \epsilon_{xy} \rangle$ at different irradiation parameters



Conclusions

Based on the phase field model in the framework of nonlinear elastic theory we have performed the three-dimensional numerical modeling of elastic fields evolution for shear deformation of binary Zr-10%Sn alloy and have studied irradiation and strain rate influence on the mechanical properties change.

We have found that:

- the growth of strain rate from $10^8 s^{-1}$ to $10^9 s^{-1}$ leads to the increasing of the resistance of alloy to plastic deformation and to its hardening for both unirradiated and irradiated one, due to the increase in the yield strength and ultimate strength with the strain rate;
- the yield strength and ultimate strength increase with the irradiation dose rate and decrease with irradiation temperature;
- the growth of irradiation dose to 2 *dpa* results in the increasing of the yield strength and ultimate strength;
- the transition toward negative values of strain hardening coefficient, that is related to deformation softening, is realized later, that is at larger values of strain, for previously irradiated samples.

Obtained results allows to establish the deformation processes of internal stresses and strains redistribution in the bulk, to determine the general patterns of change in mechanical properties of Zr-Sn alloys under irradiation, that is important to predict the reliability and endurance of alloy.

References

1. A. Minami and A. Onuki, *Phys. Rev. B*, **72**: 100101 (2005).
2. A. Minami and A. Onuki, *Acta Materialia*, **55**: 2375 (2007).

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