Power uprates
and plant life extension

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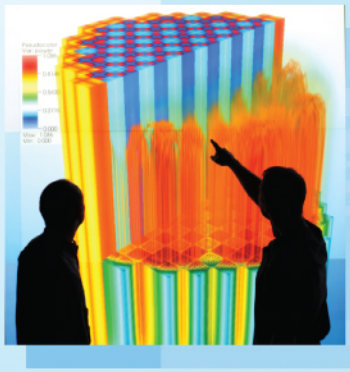
Consortium for Advanced Simulation of LWRs



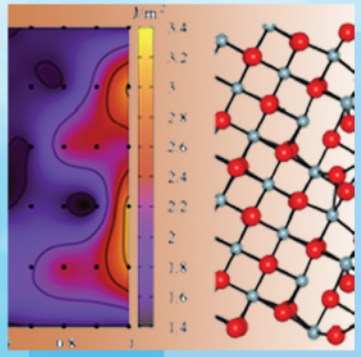
Engineering design
and analysis

Generalization of the ORNL Radiation Growth Model for Zr-Based Materials to Account for Internal and External Stresses

Science-enabling
high performance
computing

Stas Golubov, Sasha Barashev, and Roger Stoller

Oak Ridge National Laboratory



Fundamental science

April 12, 2013

Plant operational data

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Generalization of the ORNL Radiation Growth Model for Zr-Based Materials to Account for Internal and External Stresses

L3:MPO.CLAD.P6.01

Stas Golubov
Sasha Barashev
Roger Stoller

Materials Science and Technology Division
Oak Ridge National Laboratory

MPO meeting
Oak Ridge
April 12 - 2013

Managed by UT-Battelle
for the Department of Energy

CASL-U-2013-0091-000

OUTLINE

- Radiation growth and creep
- Creep via climb-assistant glide
- Incorporation of the creep model to VPSC
- Future work

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Radiation Growth Problem

The first Radiation Growth model was suggested at **1962 (Buckley)** (several years before swelling was discovered)

Many models have been proposed since then, however

'.... reliable mechanistic models to predict the deformation of even a pure Zr single crystal are not known ... We therefore still rely on a phenomenological approach.'

Holt, *J. Nucl. Mater*. 372 (2008) 182.

... understanding of the basic creep mechanisms in anisotropic materials like zirconium alloys is still not strong enough to be truly predictive.' ... Today, most models are empirical in nature ...

Adamson *et al, Advance Nuclear Technology International* (2009).

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Radiation Growth and Creep

- Many models have been developed during last 50 years for RG and RC without accounting for the possible connections between them
- However there is **one case only** where the separation of RG and RC has sense: **RG in unstressed single crystals**
- RG in unstressed multigrain materials is always accompanied with RC
- In multigrain materials under external stress, that is the case of practical interest, **RG and RC operates simultaneously**

Such approach has never been used

Implementation of RG model developed at ORNL to describe creep in VPSC code developed at LLAN-
the first attempt to build physical based predictive description of dimensional instability of Zr-based alloys

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New RG model for Zr

In Cartesian system with *x* and z axis parallel to a_1 and *c* directions the RG strain rates are given by:

$$\frac{d\varepsilon_x}{d\phi} = \chi\left(\frac{1}{2} - \frac{\rho_x}{\rho}\right),$$

$$\frac{d\varepsilon_y}{d\phi} = \chi\left(\frac{1}{2} - \frac{\rho_y}{\rho}\right), \qquad \phi = Gt,$$

$$\frac{d\varepsilon_z}{d\phi} = -\chi\frac{\rho_z}{\rho}.$$

***X* - properties of cascades,**

ρ_x/ρ, ρ_y/ρ, ρ_z/ρ - fractions of *c*- and *a*- dislocations

S.I. Golubov, A.V. Barashev, and R.E. Stoller, On the Origin of Radiation Growth of HCP Crystals, ORNL/TM-2011/473.

Microstructure evolution

$$\rho_{x,y,z}(\phi) = \rho_x(0) + 2\pi R_{x,y,z}(\phi) N_{x,y,z}(\phi)\ ,$$

$R_{x,y,z}(\Phi)$, $N_{x,y,z}(\Phi)$ are radius and density of dislocation loops, $\Phi = \phi t$ is fluence

A.V. Barashev, S.I. Golubov, R.E. Stoller. Theoretical Investigation of Microstructure Evolution and Deformation of Zirconium under Cascade Damage Conditions, ORNL/TM-2012/225.

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The RG model explains and predicts:

- Strain saturation and breakaway
- Negative *a*-strain
- Coexistence of vacancy and SIA prismatic loops
- Estimate of strain rate at high doses, i.e. to where the breakaway goes

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Dose dependence of RG

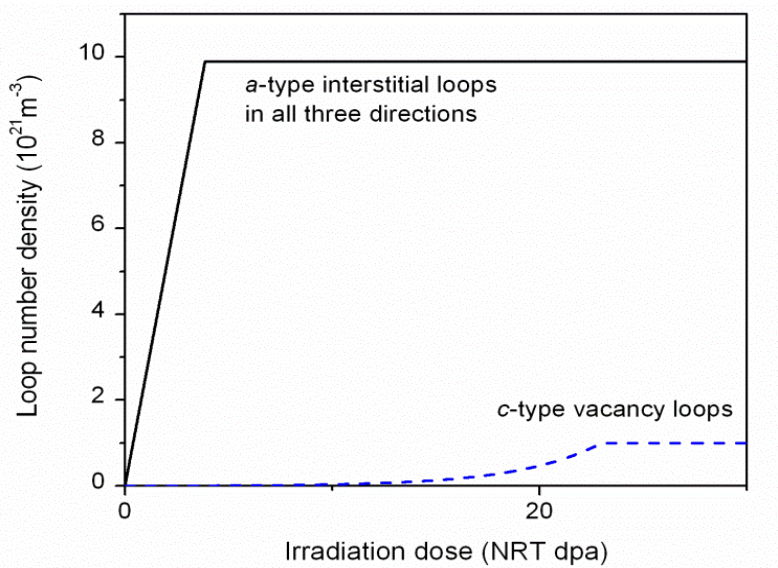
$$\rho_{x,y,z}(\phi) = \rho_{\mathrm{x}}(0) + 2\pi R_{x,y,z}(\phi) N_{x,y,z}(\phi)\ ,$$

$R_{x,y,z}(\Phi)$, $N_{x,y,z}(\Phi)$ are radius and density of dislocation loops

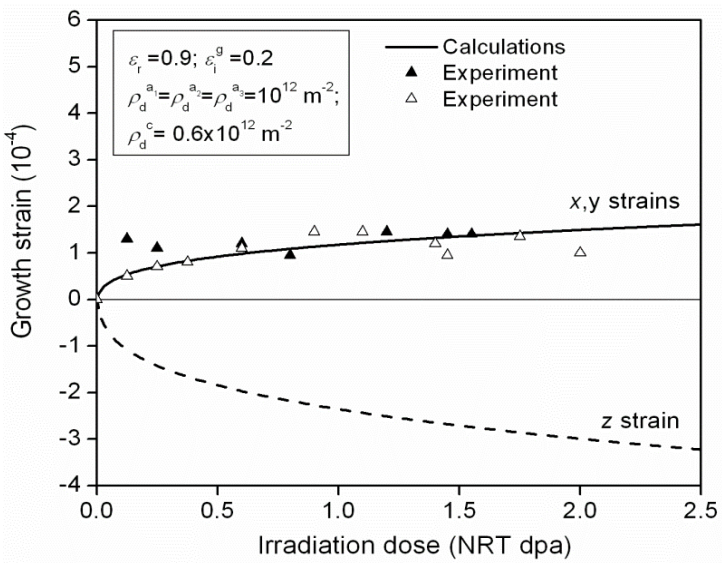
$\phi = Gt$ is fluence

Mechanisms of dislocation loop nucleation are not known

Phenomenological approach

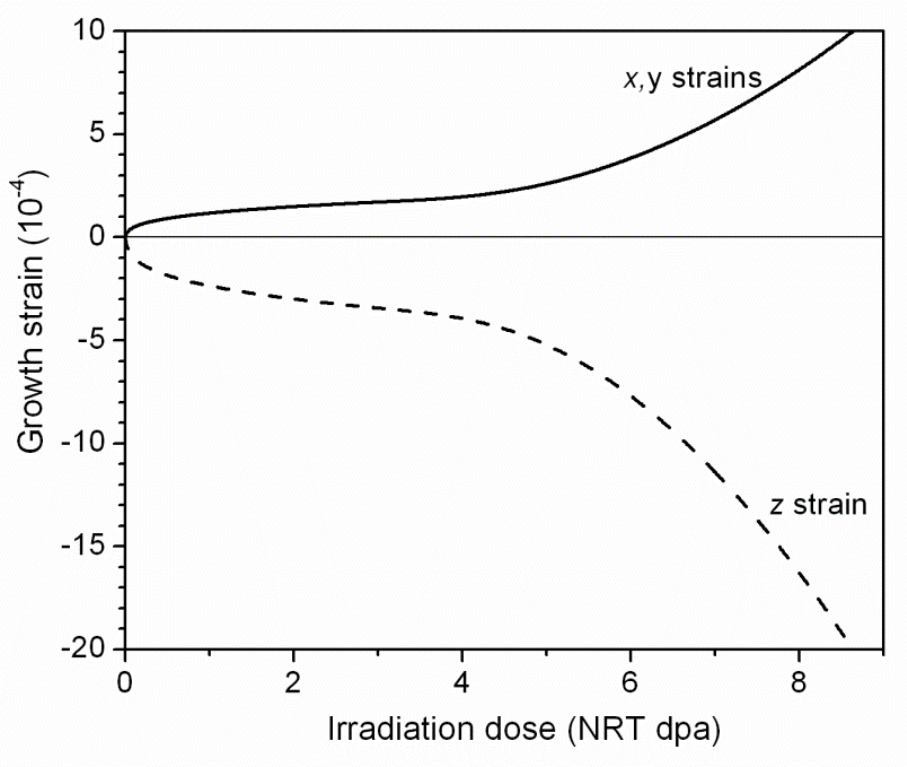


Dependence of vacancy and interstitial loop number densities on the irradiation dose.



Comparison of the calculated growth strain and experimental measurements.

Radiation growth of annealed pure Zr at intermediate doses



Dose dependence of growth strain for prismatic (x,y) and basal directions (z)

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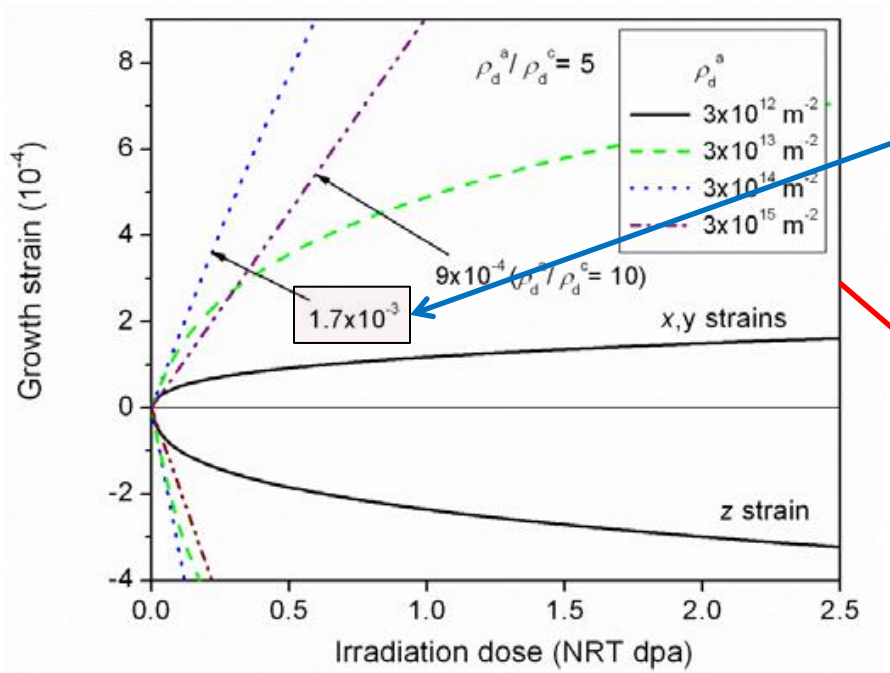
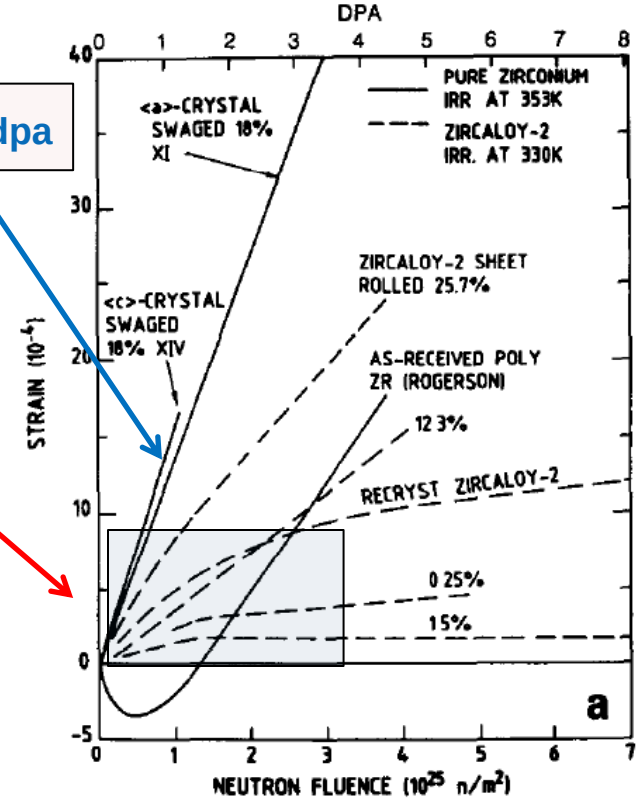
Impact cold work on dose dependence of RG



~ 10^{-3}/dpa

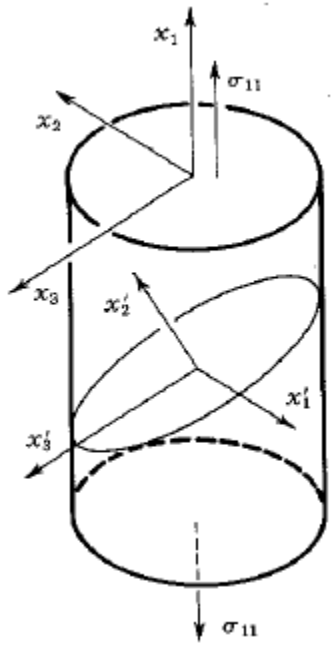


Calculated dose dependence of RG at different dislocation densities

G.J.C. CARPENTER, R.H. ZEE and A. ROGERSON
J. Nucl. Mater. 159 (1988) 86

The calculation results reproduce experiment qualitatively and quantitatively

Deformation via RG and creep, I

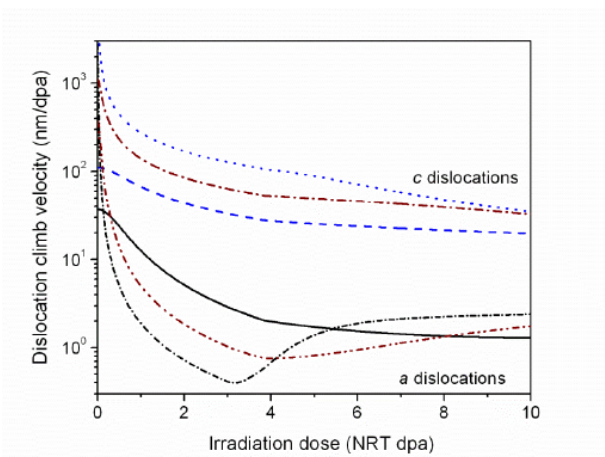


Resolve shear stress

$$\sigma_{ij} = \begin{vmatrix} \sigma_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix} \quad \Rightarrow \quad \sigma'_{1,2} = \left(\cos\alpha\cos\beta\right)\sigma_{11}$$

Shear strain due to climb-assistant glide (Gittus model) in crystallographic coordinate system

$$\frac{d\varepsilon_j^{sh}}{d\phi} \approx \frac{\sqrt{\pi}\rho_j V_j}{\mu\sqrt{\rho}}\left(\sigma'_{1,2}\right)_j, \quad (j = a_1, a_2, a_3, c)\ .$$



Total strain In crystallographic coordinate system

$$\frac{d\varepsilon_j^n}{d\phi} + \frac{d\varepsilon_j^{sh}}{d\phi} \Rightarrow \frac{d}{d\phi}\left[\begin{vmatrix} \varepsilon_{11}^n & \varepsilon_{12}^{sh} & \varepsilon_{13}^{sh} \\ \varepsilon_{21}^{sh} & \varepsilon_{22}^n & \varepsilon_{23}^{sh} \\ \varepsilon_{31}^{sh} & \varepsilon_{32}^{sh} & \varepsilon_{33}^n \end{vmatrix}\right],$$

Deformation via RG and creep, II

Euler transformation to original coordinate system

$$\left\{ \frac{d}{d\phi} \begin{vmatrix} \varepsilon_{11}^{n} & \varepsilon_{12}^{sh} & \varepsilon_{13}^{sh} \\ \varepsilon_{21}^{sh} & \varepsilon_{22}^{n} & \varepsilon_{23}^{sh} \\ \varepsilon_{31}^{sh} & \varepsilon_{32}^{sh} & \varepsilon_{33}^{n} \end{vmatrix} \right\}_{cr-sys} \Rightarrow \left\{ \frac{d}{d\phi} \begin{vmatrix} \tilde{\varepsilon}_{11}^{n} & \tilde{\varepsilon}_{12}^{sh} & \tilde{\varepsilon}_{13}^{sh} \\ \tilde{\varepsilon}_{21}^{sh} & \tilde{\varepsilon}_{22}^{n} & \tilde{\varepsilon}_{23}^{sh} \\ \tilde{\varepsilon}_{31}^{sh} & \tilde{\varepsilon}_{32}^{sh} & \tilde{\varepsilon}_{33}^{n} \end{vmatrix} \right\}_{orig-sys}$$

Dose dependence of dimensional change is described by the diagonal matrix elements of strain tensor obtained by integration over irradiation dose

$$\tilde{\varepsilon}_{11}^{n}(\sigma,\phi)\ ,\tilde{\varepsilon}_{22}^{n}(\sigma,\phi)\ ,\tilde{\varepsilon}_{33}^{n}(\sigma,\phi)\ .$$

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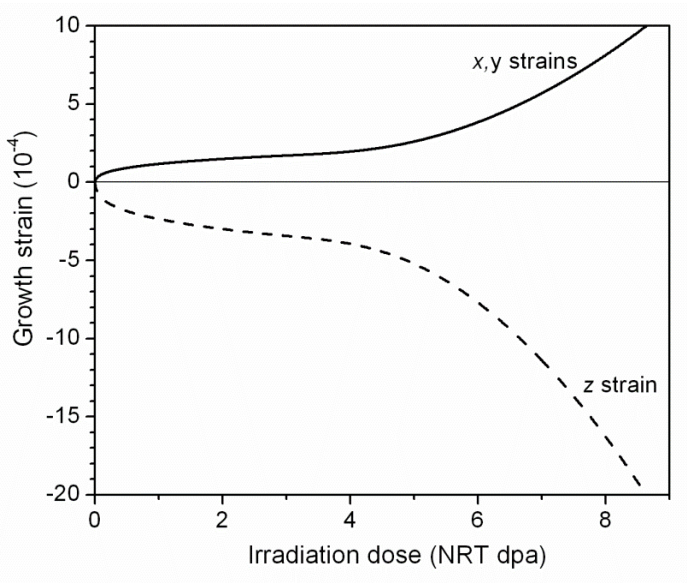
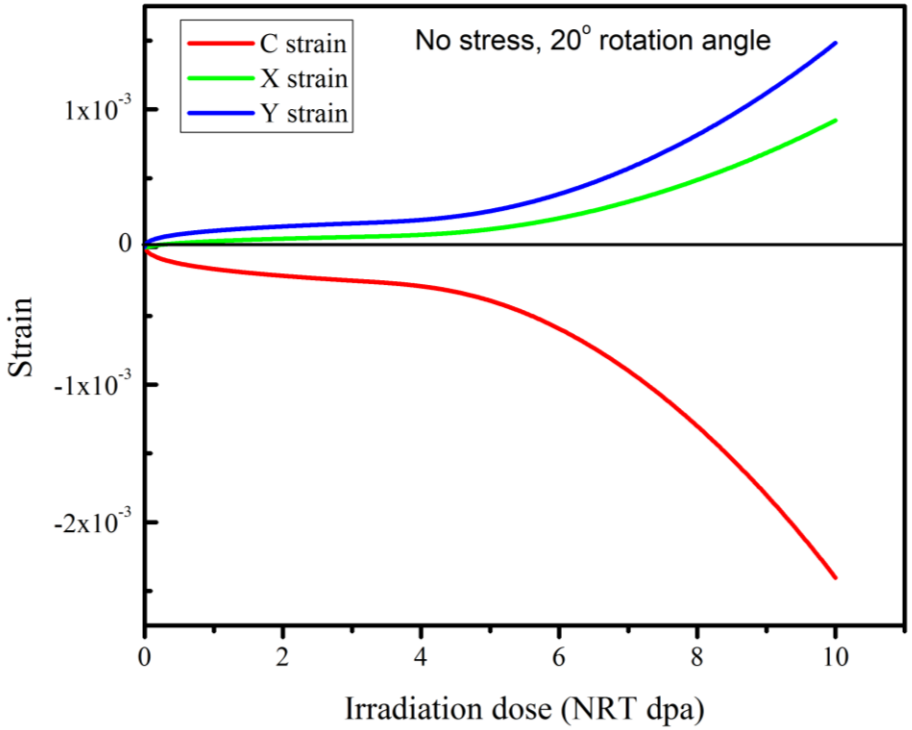
Dose dependence of strain of annealed single crystal of Zr via RG

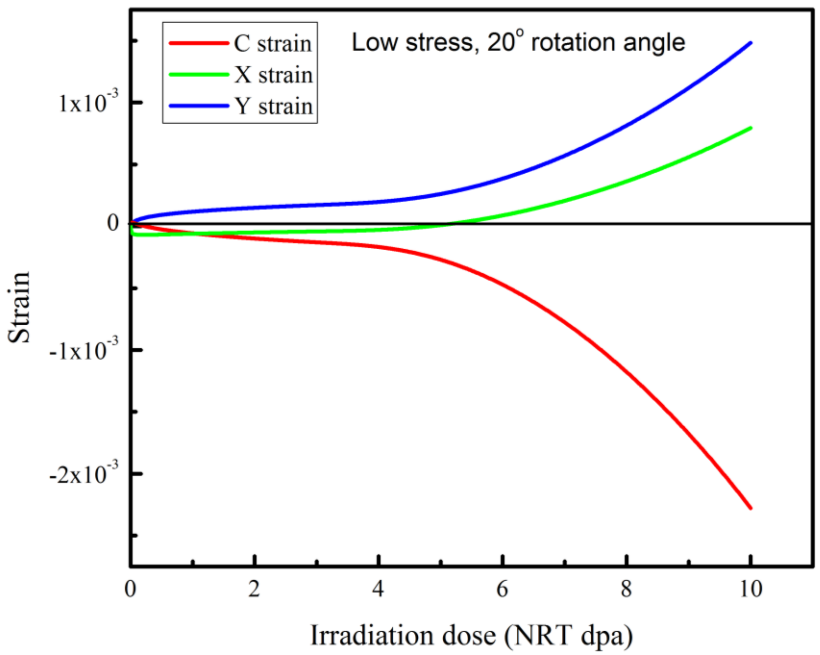
Crystallographic system

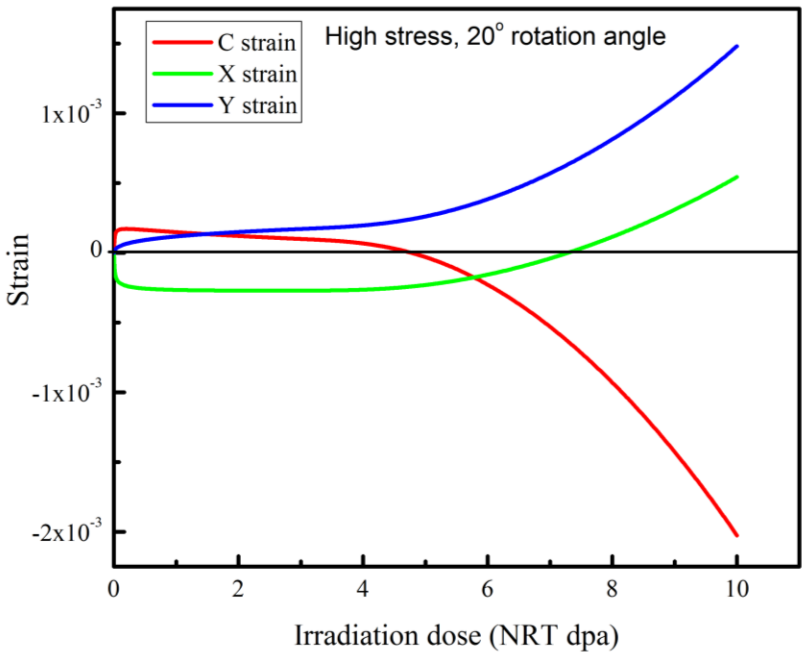


Original system (rotation along y-axis)

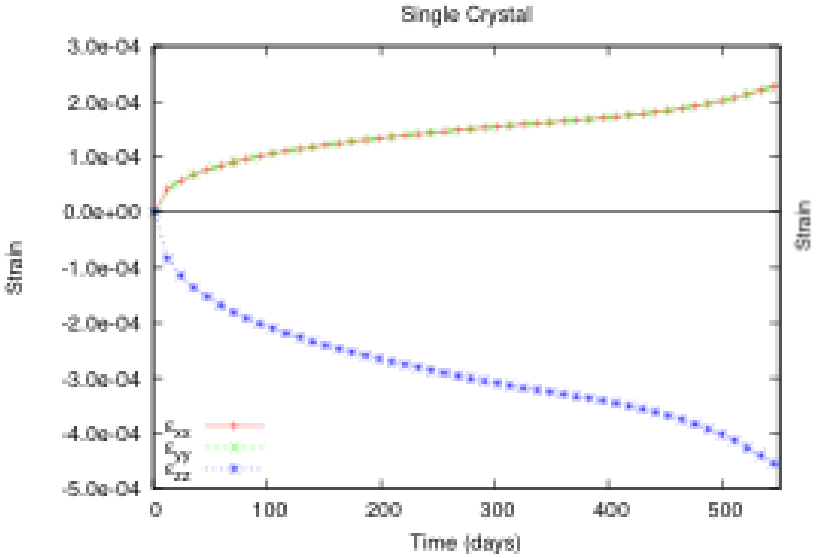


Dose dependence of strain of annealed single crystal of Zr via RG & creep

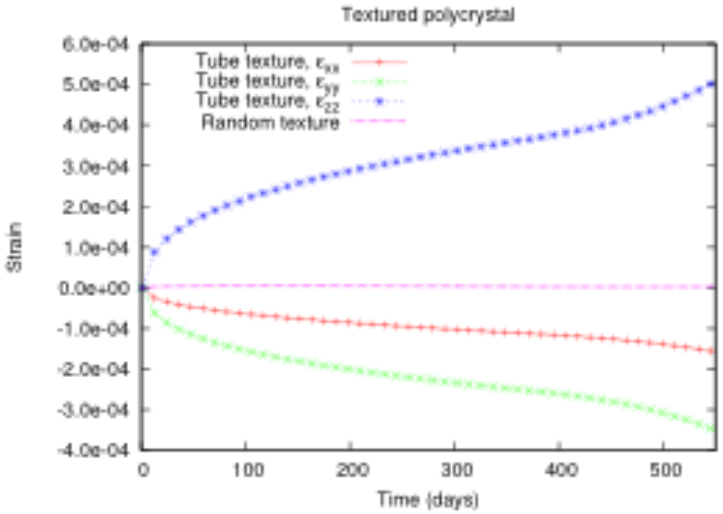


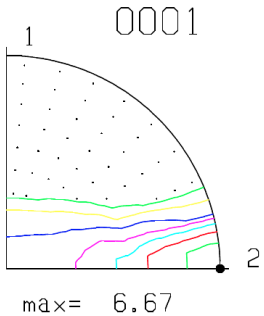


An example of coupling RG and VPSC models



Dose dependence of RG strain in single Zr crystal





Dose dependence of strain in textured polycrystalline Zr via RG and creep described by a phenomenological

Implementation of Gittus model based on ORNL RG model to the LLNL VPSC code is in progress

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2013: Further work

- **Detail study of deformation of Zr materials due to radiation growth and creep in single and multigrain crystals**

- **Account for impact of grain boundaries on deformation of Zr materials**

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End of presentation.

Thanks for your attention

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