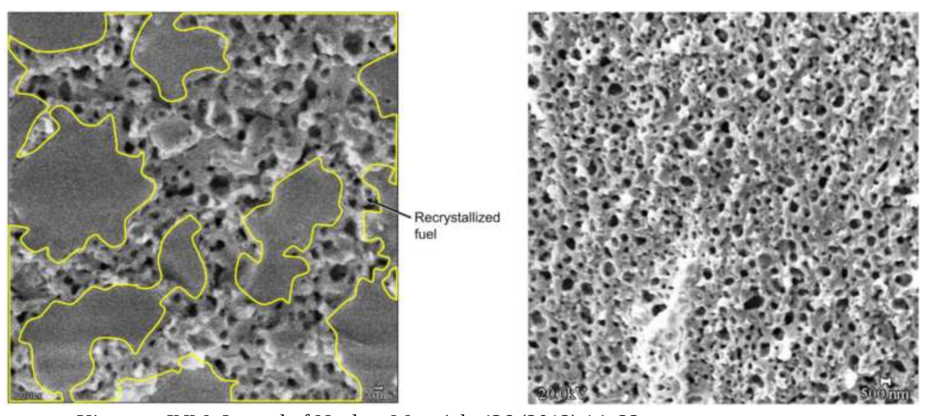
Mesoscale Modeling of High Burn-up Structure (HBS) Formation and Evolution in Metallic Fuels

M. Gomaa Abdoelatef[1], F. Badry[1], Karim Ahmed[1], Sudipta Biswas[2], Andrea Jokisaari[2], Daniel Schwen[2], Yongfeng Zhang[2], Cody Permann[2]

[1] Nuclear Engineering Department, Texas A&M University, College Station, TX, USA.
[2] Fuel Modeling and Simulation Department, Idaho National Laboratory, Idaho Falls, ID, USA.

Introduction

- U-7Mo and other nuclear fuels develop a unique microstructure under **irradiation** usually known as the High Burn-up Structure (**HBS**)
- In this **HBS**, the as-fabricated microstructure transforms into a much finer one with a grain size that is orders of magnitude less than the initial grain size.
- The **increase** in the free energy due to the **formation** of new grain boundaries is **offset** by the reduction in the free energy by creating **dislocation-free** grains at the expense of the deformed grains.
- **Recrystallization** was proposed as a mechanism that **facilitates** HBS formation.



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- It was shown that the **HBS** formation alters the **swelling** and **gas release** rates, and hence affects the fuel **integrity and performance**. Therefore, investigating the formation and evolution of the **HBS** in nuclear fuels is of paramount importance for enhancing the reactor **performance** and **safety**.
- This figure shows SEM images of atomized U–10Mo showing evolution of recrystallization with fission density. The bubbles nucleate first and then new sub-grains nucleate around the bubbles and original grain boundaries.
- We utilize here a **phase field** model to study **irradiation-induced** recrystallization.

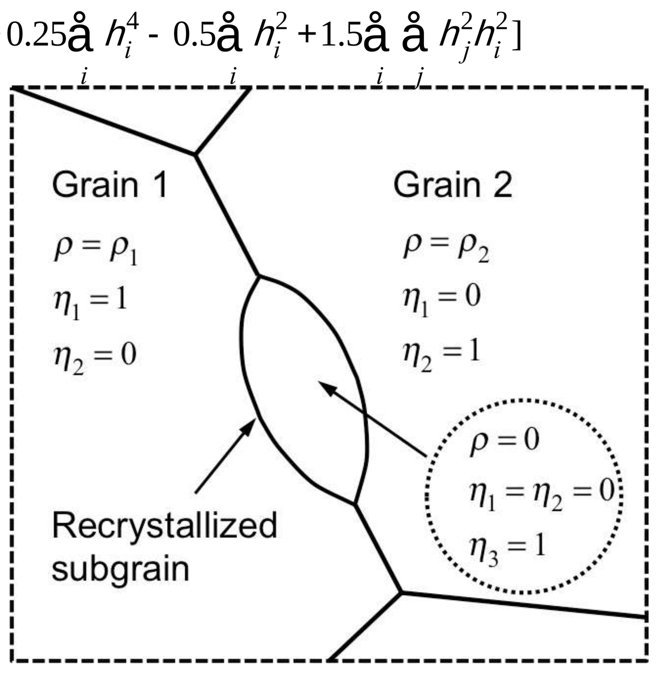
Phase Field Model

- The total **free energy** of the system is given by

$$F=\int f(\eta_1,\dots,\eta_p)+g(\rho_{\mathrm{eff}},\eta_1,\dots,\eta_p)+\frac{1}{2}\sum_{\alpha=1}^{p}\kappa_\eta\left|\nabla\eta_\alpha\right|^2 \quad d^3r$$

- The **effective** dislocation density is calculated as, $\rho_{\mathrm{eff}}=\dfrac{\sum_i \rho_i\eta_i^2}{\sum_i \eta_i^2}$
- The **stored energy** associated with dislocations has the form, $g(\rho_{\mathrm{eff}},\eta_1,\dots,\eta_p)=\frac{1}{2}\mu b^2\rho_{\mathrm{eff}}$, and the Landau polynomial is the same as in grain growth models, e.g.,

$$f(\eta_1,\dots,\eta_p)=A[0.25+0.25\sum_i\eta_i^4-0.5\sum_i\eta_i^2+1.5\sum_i\sum_j\eta_j^2\eta_i^2]$$



A schematic illustration of the order parameters used in the phase-field model.

- The **non-conserved** order parameters representing the **grains** are then evolved via **Allen-Cahn** dynamics,

$$\frac{\partial\eta_\alpha}{\partial t}=-L\left[\frac{\partial f(\eta_1,\dots,\eta_\alpha,\dots,\eta_p)}{\partial\eta_\alpha}+\frac{\partial g(\rho_{\mathrm{eff}},\eta_1,\dots,\eta_\alpha,\dots,\eta_p)}{\partial\eta_\alpha}-\kappa_\eta\nabla^2\eta_\alpha\right]\quad\forall\,\alpha,\ \alpha=1,2\dots p$$

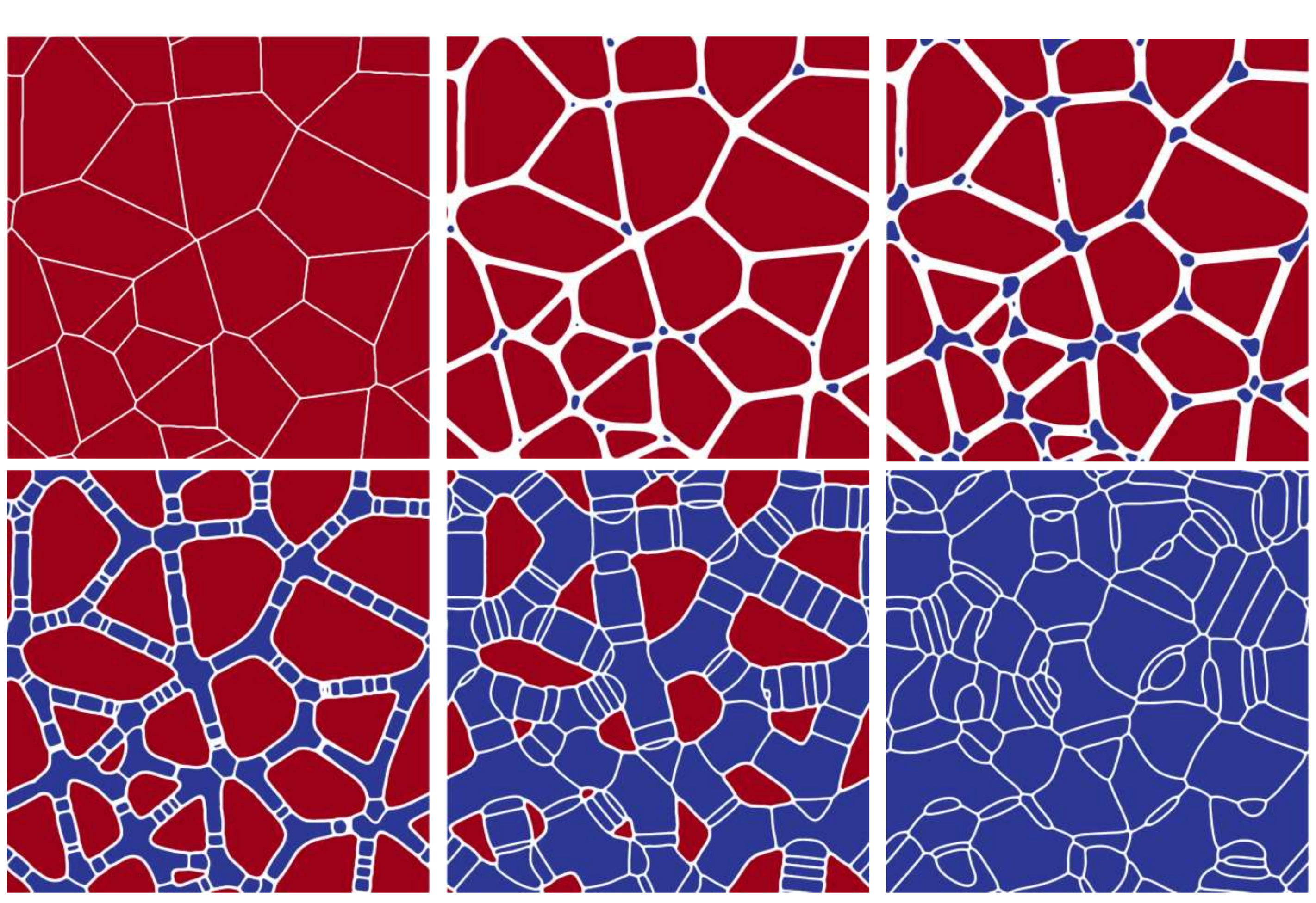
- The model **parameters** are directly related to the grain boundary **energy** and **mobility** as

$$A=\frac{3\gamma_b}{4\ell},\quad \kappa_\eta=\frac{3}{4}\gamma_b\ell,\quad L=\frac{4M_b}{3\ell}$$

- The kinetic equations are solved via a fully-coupled, fully-implicit **finite-element** scheme implemented in the Multiphysics Object Oriented Scientific Environment (**MOOSE**) code.
- We use **Grain Tracker** algorithm to represent **many** grains with a **few** order parameters.

Results

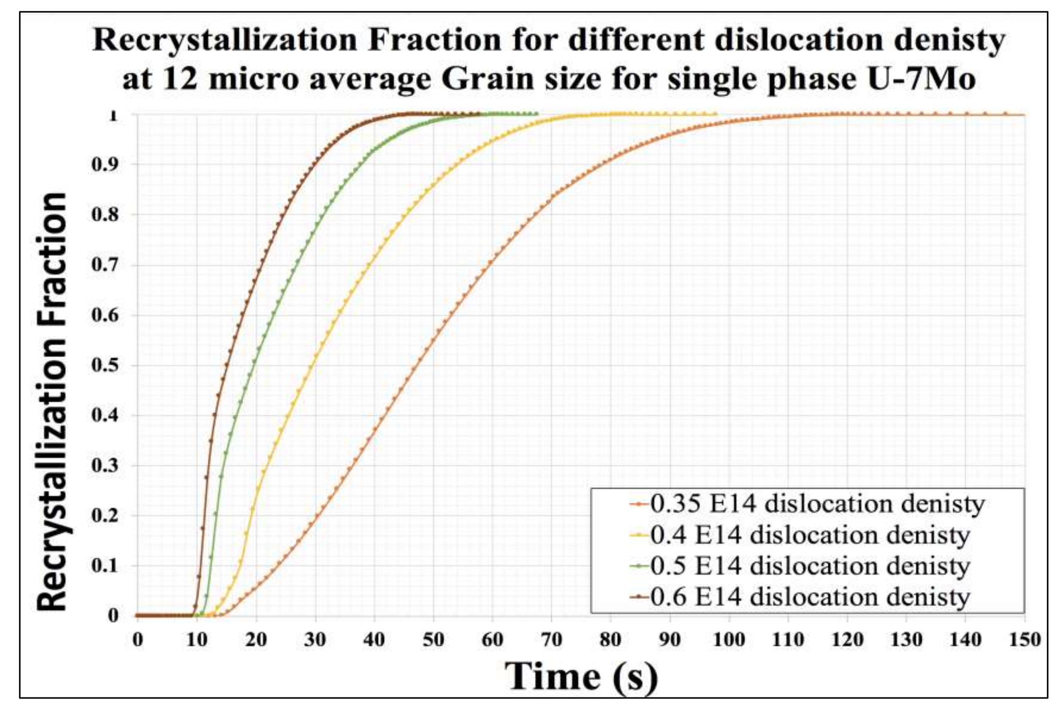
- The recrystallized grain, grows **only if** the dislocation density in the deformed grain is higher than a **critical** value given by $\rho^c=\dfrac{2\gamma_b}{\mu b^2R}$
- We have carried out several 2D simulations for investigating the irradiation-induced recrystallization. We present and discuss the results of recrystallization behavior of U-7Mo in two cases.
- First case, single phase U-7Mo, which we study the recrystallization rate of a recrystallized grains against different grain sizes (at $0.4x10^{14}cm^{-2}$ *dislocation denisty*) and different dislocation densities (at 12 μm average grain size).

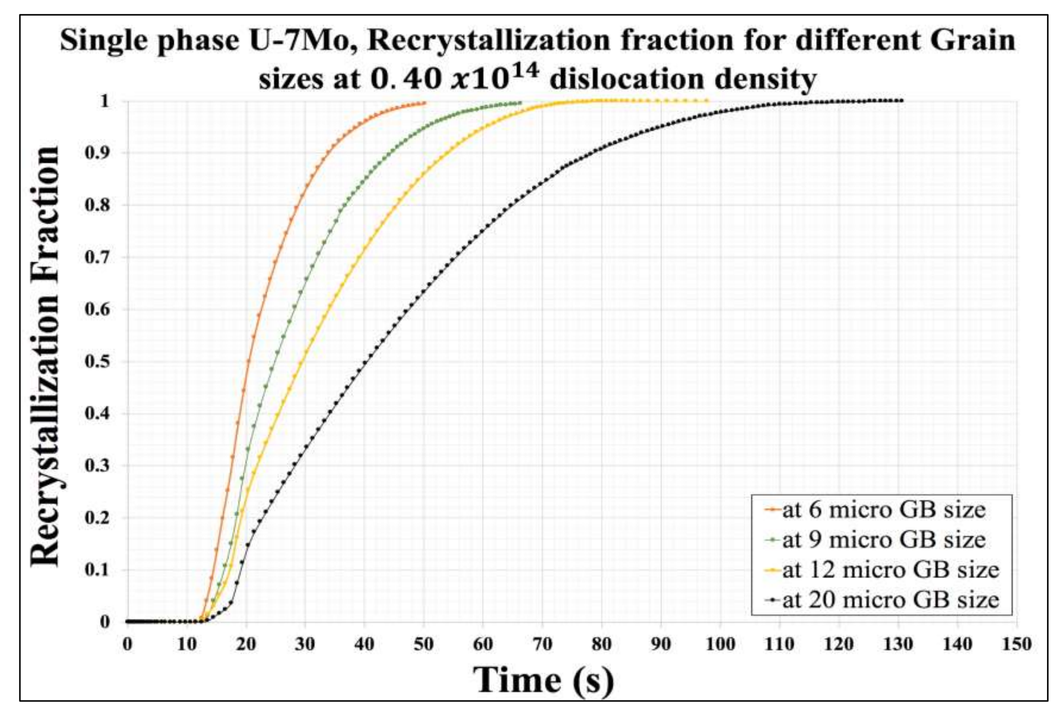


Results (cont'd)

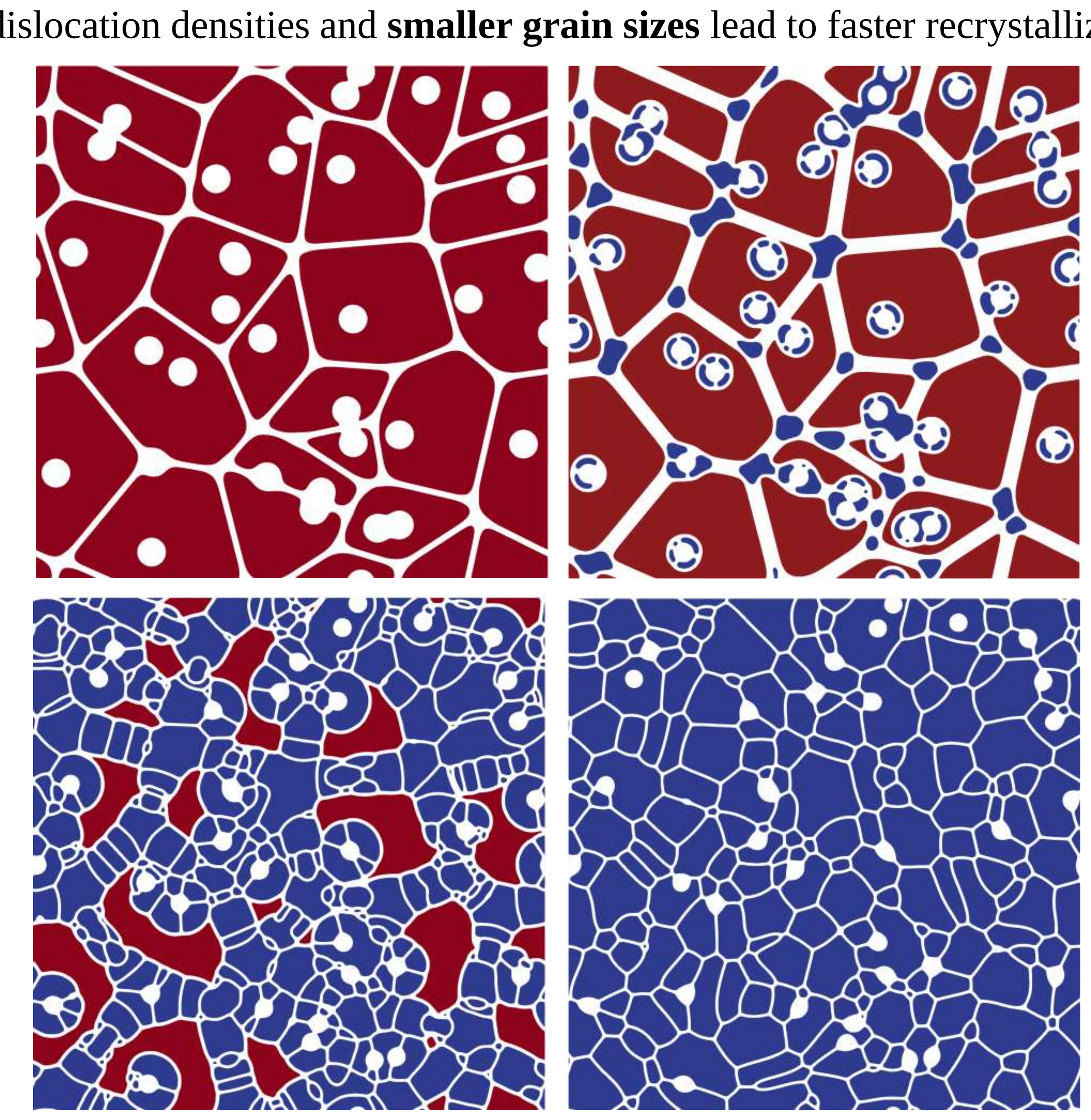
Snapshots of single phase polycrystalline U-7Mo structure (left upper figure) with both damaged (in red) and recrystallized (in blue) grains. Sub-grains nucleate on the triple-junction and on the grain boundaries.

Recrystallization progress for a single phase U-7Mo in the two cases. First, at different dislocation density (right upper figure) with 12 micro meter average grain size. Second, at different grain sizes (right down figure) with $0.4x10^{14}cm^{-2}$ *dislocation denisty*. The recrystallization behavior in the two cases, illustrate that **Higher** dislocation densities and **smaller grain sizes** lead to faster recrystallization rate.

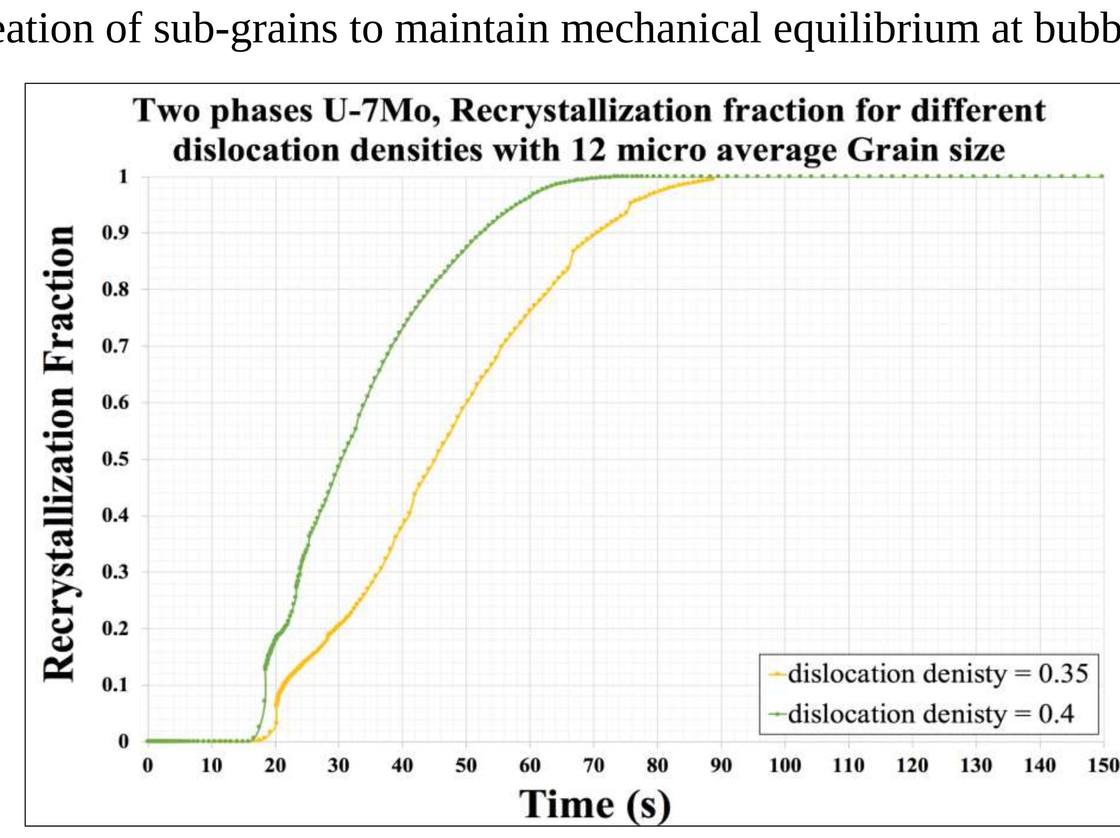




- Second, in case of existing a second phase particle, we study the recrystallization rate of a recrystallized at specific grain size (12 μm) against different dislocation densities. We then investigate the irradiation-induced recrystallization in U-7Mo (formation of the HBS).
- There is a **threshold** value for the dislocation density (or equivalently Burn-up) at which recrystallization takes place. For the case of U-7Mo at 1273 Kelvin, that value is $\rho_{\mathrm{eff}}^c=0.35\times10^{14}\mathrm{m}^{-2}$.
- **Higher** dislocation densities and **smaller grain sizes** lead to faster recrystallization rate.



Snapshots of the recrystallization process in U-7Mo in the presences of bubbles. Since grain boundary energy is higher than surface energy, the sub-grains form first at the triple junctions, then grain boundaries and then bubble surface. The bubbles shape also changes after the nucleation of sub-grains to maintain mechanical equilibrium at bubble tip.



The recrystallization progress in U-7Mo in case of existing a second phase particle vs. different dislocation density. At 12 micro meter average grain size, it shows that the higher dislocation density leads faster recrystallization rate.

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