Effect of the HPTE process regimes on the recrystallization kinetic of the ultrafine-grained pure aluminum: multiphase-field model simulation and experimental validation

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Introduction.

Studying the kinetics of recrystallization (ReX) of severely deformed materials, especially at the initial stages of the process, is very important for maintaining the increased strength of ultrafine-grained materials (UFG) and determining their service properties in general and the sustainable conditions of their use in machines and mechanisms in particular. Using a digital twin of the ReX process implemented in the phase field model [1] allows us to study in detail the initial stages of ReX, which is inaccessible for experimental study due to the methodological difficulties in implementing an instant stop of the process in a bulk material. This paper presents the results of simulating the recrystallization of two states of UFG aluminum obtained by High Pressure Torsion Extrusion (HPTE) with different degrees of deformation. The effect of the accumulated degree of deformation and grain size in the UFG structure on the development of recrystallization, a drop in dislocation density and, accordingly, the softening rate is shown.

Experimental part

In this study, the ReX process of a pure aluminum rod, measuring 35 mm in length and 10.8 mm in diameter, subjected to severe deformation via HPTE [2], was investigated. Two HPTE regimes provided UFG structure formation were employed. The material underwent static annealing at 300°C for various durations, ranging from 10 minutes to 5 hours. The softening behavior induced by ReX was assessed through dislocation density measurements. Differences in ReX kinetics provided various storage energy in as-deformed states were analyzed.

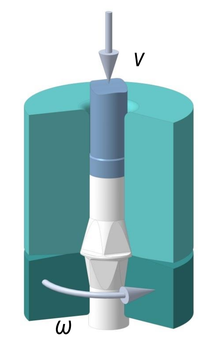
HPTE treatment

- **Material**: HPTE- processed pure Al
- **HPTE** at room temperature **regimes variation:**
  1) $\boldsymbol{v1w1}$
  2) $\boldsymbol{v1w3}$
- Strain dependence:

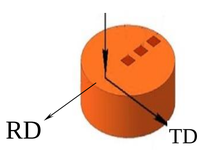
$$e \sim \frac{w * R}{V}$$

- **Static recrystallization:** isothermal, annealing at **300°C** during **10, 30, 60, 300** and **1200** min. Quenching to water.
- **Material characterization by** SEM EBSD**:**
  - Orientation image (OI) microscopy maps
  - Geometrically necessary dislocations (GND)

HPTE scheme

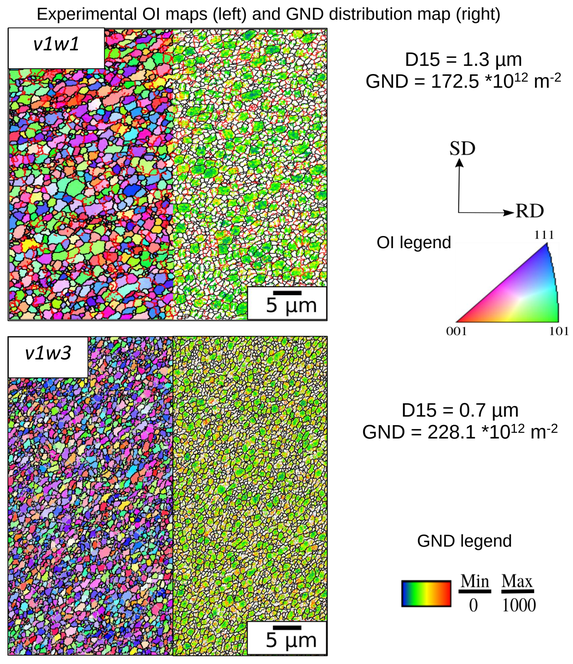


ED



As-deformed states:

Experimental OI maps (left) and GND distribution map (right)



Simulation of the recrystallization by mutiphase-field modeling

Experimentally obtained Orientation Imaging Microscopy (OIM) maps were imported for recrystallization (ReX) simulation using the multiphase-field model (PFM)

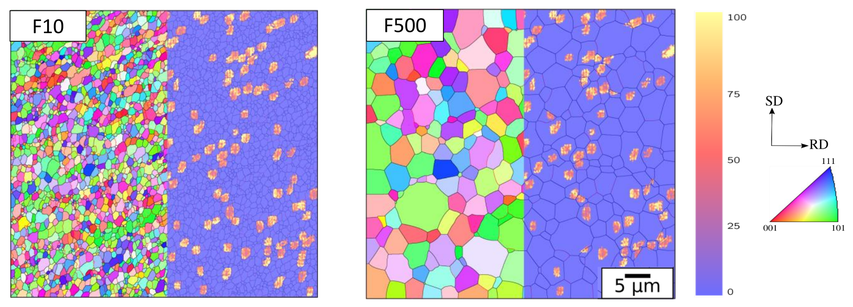
- **Simulations of ReX:** Multiphase-field Model [3,4]
- Ginzburg - Landau free energy functional

$$\mathcal{F} = \int_V \underbrace{\varepsilon a(\phi, \nabla\phi) + \frac{1}{\varepsilon}\omega(\phi)}_{W_{\text{intf}}} + \underbrace{f_{RX}(\phi, \rho_d)}_{W_{\text{bulk}}} dV,$$

Kadi4Mat and KadiStudio in Our Research

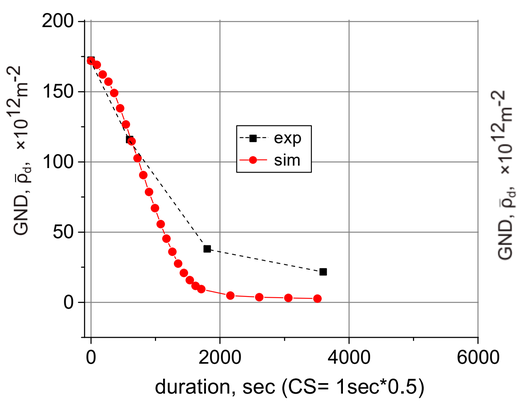
- Efficient data management: Kadi4Mat [5-7] provides a structured database for our annealing experiments on deformed aluminum, enabling easy storage and retrieval of experimental and simulation data.
- Workflow automation: KadiStudio allows us to create reproducible workflows for processing in-situ measurements and analyzing dislocation density changes, enhancing research efficiency.
- Seamless integration: These tools facilitate the integration of our experimental data with PACE 3D simulation results, allowing for more effective comparison and analysis. Enhanced collaboration: The Kadi ecosystem promotes better data sharing and collaboration among our research team, accelerating the pace of our recrystallization studies.

Simulated OI maps (left) and storage energy maps (right) v1w1

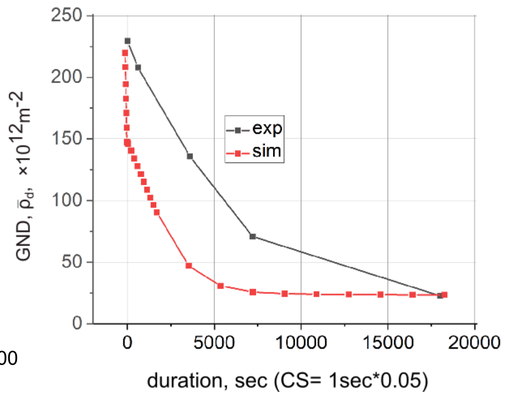


Storage energy relaxation kinetics simulation and validation

v1w1



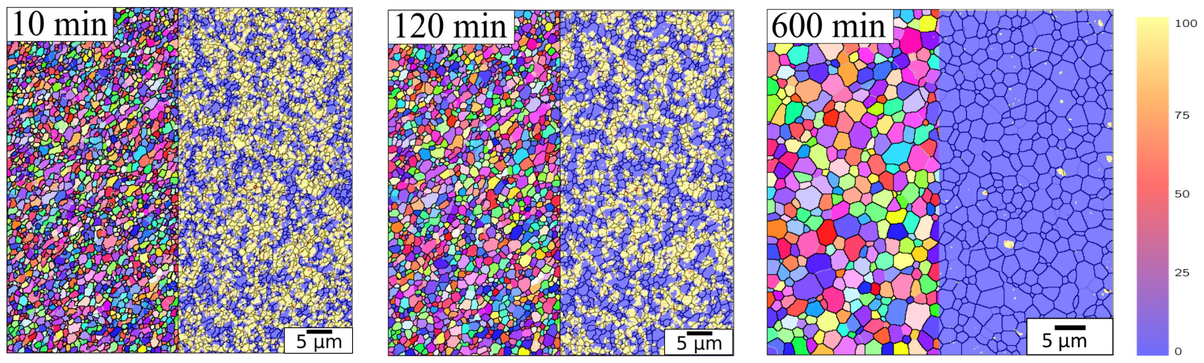
v1w3



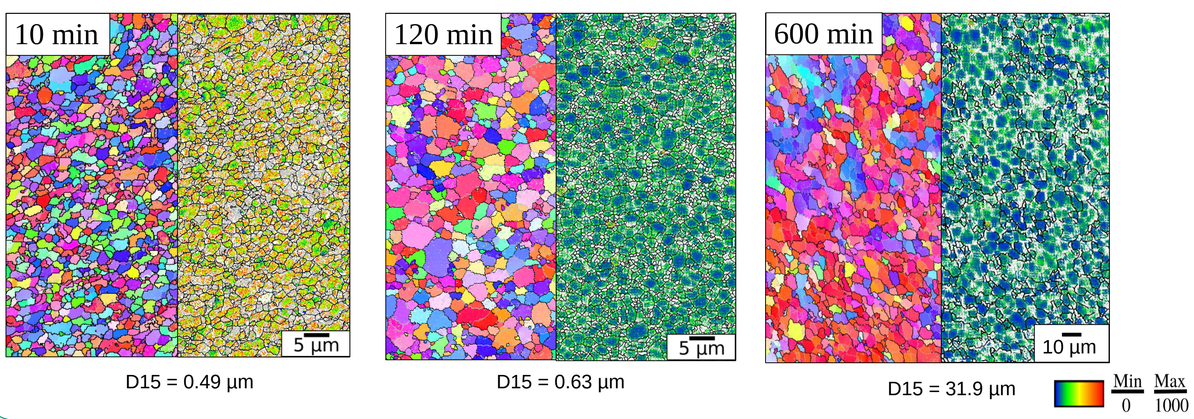
- A higher initial dislocation density and a slow rate of its fall in the structure obtained by HPTE *v1w3* were experimentally detected. For the simulation in PACE 3D, the mobility of grain boundaries $M_{\alpha\beta}$ was intentionally not changed to indicate the effect of increased dislocation density on the calculated recrystallization kinetics.
- Obviously, a higher dislocation density and, accordingly, a larger SE in the initial structure demonstrates a slower kinetics of the fall of the stored energy than for the *v1w1* mode. However, the obtained rate of fall of the calculated GND values significantly exceeds the experimentally observed rate of fall.

Experimental and simulation structure evolution during the ReX process after HPTE *v1w3*

Simulated OI maps (left) and storage energy maps (right)



Experimental OI maps (left) and GND distribution (right)



Summary and outlook

- The HPTE regime *v1w3* provides a significantly higher accumulated dislocation density and a smaller grain size in the microstructure of the pure aluminum, than processing with the *v1w1* regime at room temperature.
- The values of $\gamma_{\alpha\beta}$ and $M_{\alpha\beta}$ adopted for the MPFM calculation provide a recrystallization kinetics of the *v1w1* structure close to the experimentally observed kinetics. However, for *v1w3*, these same parameters of grain boundary mobility provide a significantly faster loss of the energy stored in the form of dislocation density. In this case, grain growth occurs much more slowly than that observed experimentally obtained.

Acknowledgment

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