The manufacturing of superconducting radio frequency (SRF) cavities for particle accelerators is currently transitioning from high-purity rolled sheet Nb to large grain Niobium (Nb) directly cut from ingots. Cavity forming from large grain disks with inherent mechanical anisotropy results in non-uniform deformation and causes defects that can limit cavity performance. To predict how dislocation density can recover and influence recrystallization, the ability to accurately model dislocation evolution during deformation is required. To this end, a constitutive crystal plasticity model for plastic deformation in Nb has been formulated by incorporating dislocation interactions and the thermally activated character of screw dislocation motion.

Design of uniaxial deformation experiments

- A high-purity Nb disk with 10 large grains was used in this study.
- Inverse pole figures (IPFs) are used to visualize the crystallographic orientations parallel to the direction of tensile deformation.
- A software toolbox was developed to calculate and visualize the Schmid factors for each slip system across the different single crystal orientations resulting from the anticipated loading.
- This allows to identify regions within the IPF for which different combinations of (1 1 0) and (1 1 2) planes constitute the most active and second-most active slip family.
- In this study, three orientations (marked red in the IPF) have been chosen for analysis based on expectation of slip system activation.

Constitutive modeling of niobium

- The crystal plasticity simulations are based on a finite strain framework.
- The plastic velocity gradient is additively composed of individual slip contributions on planes with normal n along directions m:

  \[ \mathbf{\dot{v}} = \sum \mathbf{\dot{v}}^n \mathbf{m} \otimes \mathbf{m} = \sum \mathbf{\dot{v}}^\alpha \mathbf{P}^\alpha \]  

- Each slip rate follows as the product of Burgers vector magnitude \( \mathbf{b} \), dislocation density \( \varphi \), and the dislocation velocity \( \mathbf{v} \) (Orowan’s equation):

  \[ \mathbf{\dot{\varphi}} = \mathbf{b} \mathbf{v} \]  

- At low and medium temperatures and strain rates, screw dislocation motion is the rate-limiting step in bcc metals and proceeds via nucleation (width \( \lambda_\parallel \)) of kink pairs that advances the dislocation by \( \lambda_\parallel \) in time \( t_\parallel \):

  \[ \mathbf{v} = \mathbf{b} \frac{\lambda_\parallel}{t_\parallel} = \mathbf{b} \frac{\lambda_\parallel}{t_\parallel} = \frac{2 \mathbf{b} h \tau_\parallel \mathbf{m} \otimes \mathbf{m}}{4 \mathbf{b} h \tau_\parallel \mathbf{m} \otimes \mathbf{m}} \exp \left( \frac{-\Delta \mathbf{H}}{k_B T} \right) \]  

- The mobile dislocation density on any slip system \( \alpha \) evolves as:

  \[ \varphi^\alpha = \varphi^\alpha \pm \frac{\mathbf{b} \mathbf{v} \mathbf{m} \otimes \mathbf{m}}{\mathbf{P}^\alpha} \]  

- Dislocation interactions (e.g. junction formation) diminish the resolved shear stress that drives dislocation motion:

  \[ \tau^\alpha = \tau^\alpha - \tau_\parallel = \mathbf{P}^\alpha \mathbf{m} \otimes \mathbf{m} - \mu b \sum \mathbf{\varepsilon}_{\alpha} \xi_{\alpha} \]  

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References