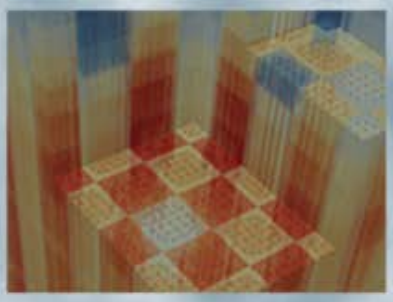
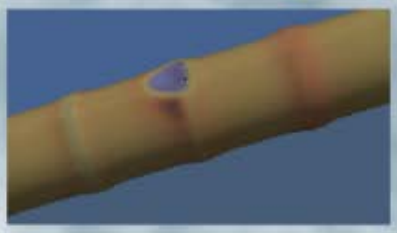
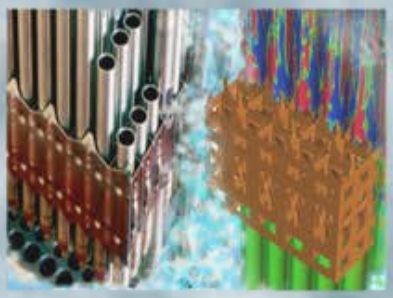
CASL-U-2015-0246-000

High Temperature Fracture Behavior of Zircaloys Materials Processing and Optimization (MPO)







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U.S. DEPARTMENT OF ENERGY | Nuclear Energy

High Temperature Fracture Behavior of Zircaloys
Materials Processing and Optimization (MPO)

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BACKGROUND AND RESEARCH OBJECTIVES

- **Pellet Clad Interactions (PCI)**
  - **Oxidation of Zr alloys leads to hydride pockets, void formation: hydride cracking and weakening of cladding**
  - **Fission products lead to interactions resulting in point defects, dislocation-densities, interstitials, swelling of cladding lead to void formation: SCC, ductile fracture**
- **Identify dominant microstructural thermo-mechanical mechanisms that globally control hydride fracture in Zr alloys: couple crystalline plasticity behavior with fracture nucleation, growth, evolution**
- **Investigate effects of crystalline structure, dislocation density interactions, GB misorientations, texture, grain-shapes**
- **Predict nucleation, propagation, characterization of intergranular and transgranular fracture modes and Interactions with hydride pockets**
- **Develop dislocation density crystalline plasticity approach for collective behavior of h.c.p. matrix, twins, and hydrides**
- **Formulate coherent interfaces orientation relations (ORs) between hydrides, twins and matrix**
- **Develop new microstructurally based finite-element computational schemes for fracture/finite strain: crack nucleation/evolution**

APPROACH

- **Dislocation Density Based Crystal Plasticity Finite Element**

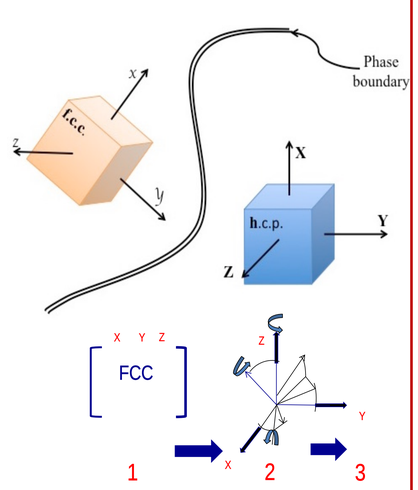
$$\rho_{tot}^{(\alpha)} = \rho_m^{(\alpha)} + \rho_{im}^{(\alpha)}$$

$$\frac{d\rho_m^\alpha}{dt} = \dot{\gamma}^\alpha\left(\frac{g_{sour}^\alpha}{b^2}\left(\frac{\rho_{im}^\alpha}{\rho_m^\alpha}\right) - g_{\min ter-}^\alpha \rho_m^\alpha - \frac{g_{immob-}^\alpha}{b}\sqrt{\rho_{im}^\alpha}\right) \qquad \frac{d\rho_{im}^\alpha}{dt} = \dot{\gamma}^\alpha\left(g_{\min ter+}^\alpha \rho_m^\alpha + \frac{g_{immob+}^\alpha}{b}\sqrt{\rho_{im}^\alpha} - g_{recov}^\alpha \rho_{im}^\alpha\right)$$

Accounts for dislocation generation, trapping of mobile dislocations, and recovery

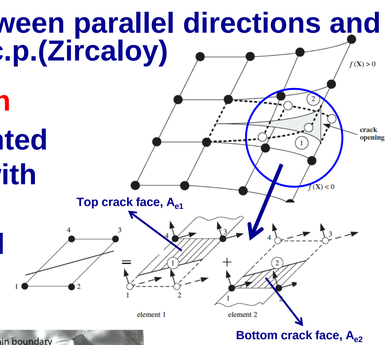
Orientation Relationships $\{0001\}_{hcp} // \{111\}_{fcc}$, $\langle 11\bar{2}0\rangle_{hcp} // \langle 1\bar{1}0\rangle_{fcc}$

- **36 ORs between f.c.c./h.c.p.**
- **Fully coherent interface between parallel directions and planes in f.c.c.(hydrides)/h.c.p.(Zircaloy)**

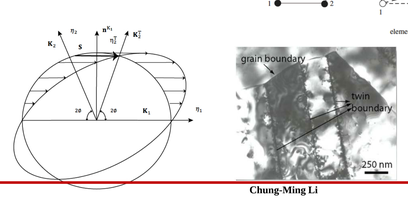


Failure surface representation

- **Fracture surfaces represented by overlapping elements with appropriate cracked area weighting of element nodal forces**



Twinning



Chung-Ming Li

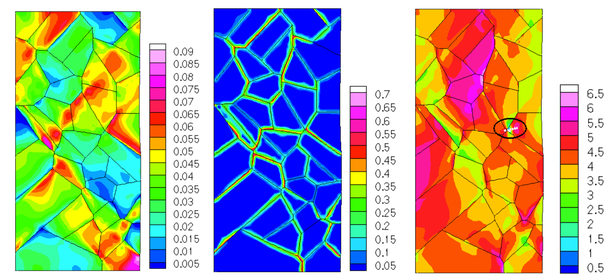
Thermo-mechanical behavior

$$\rho c_p \dot{T} = \lambda \nabla^2 T + \chi \sigma_{ij}' D_{ij}^p$$

c_p - specific heat capacity
λ - thermal conduction coefficient
χ – Quinney factor

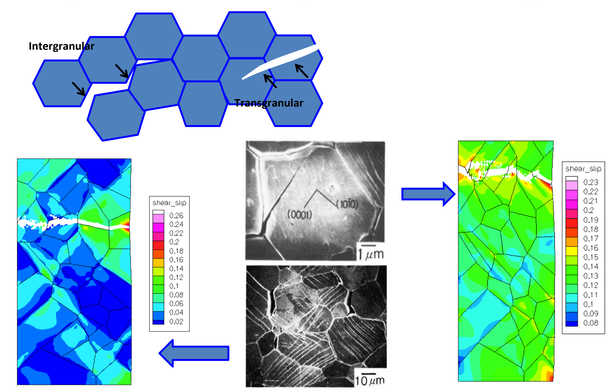
RESULTS

Slip transmission and blockage

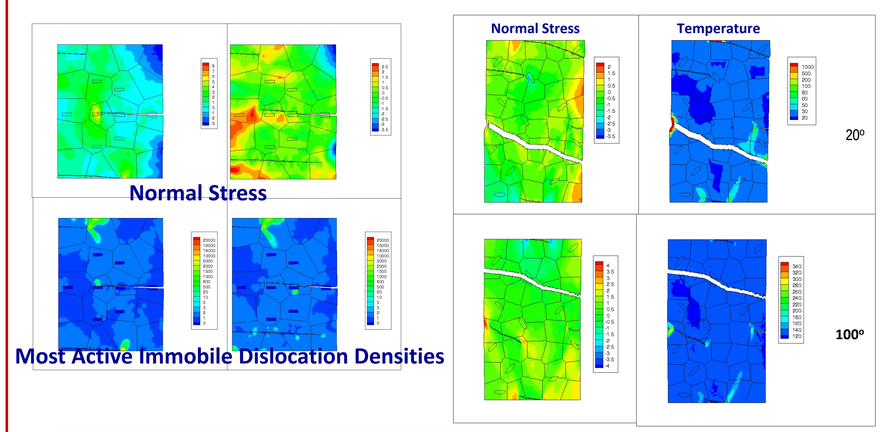


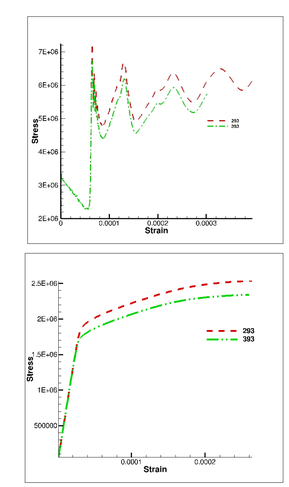
- $\rho_{junction} < 0 \rightarrow$ **Shear slip localization**
- **Slip transmission across compatible boundaries**
- **Slip blockage at incompatible boundaries**
- **Crack nucleation due to dislocation pile-up at incompatible variant boundary triple junctions**

Transgranular vs. Intergranular cracking in Zr-alloys



- **Intergranular crack path when local dislocation pile-ups result in higher stresses along the variant boundary**
- **Transgranular crack path when dislocation transmission relaxes stresses along GB boundary**





SUMMARY

- **Competition between stress buildup along basal planes and large inelastic strains on pyramidal/prismatic planes: dislocation density interactions, stress accumulation, and plastic slip behavior**
- **Transgranular crack paths when dislocation transmission relaxes stresses along GBs: low angle GB misorienations and basal plane**
- **Intergranular fracture when dislocation-pile-ups and triple junctions dominate: more likely with high angle GB misorienations, pyramidal planes**
- **Orientation Relations can accurately represent non-planar crack behavior**
- **Thermo-mechanical behavior results in different crack nucleation and softer material**

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