Constitutive Behavior Modeling

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Outline

- Constitutive behavior modeling
- Hardening models
- Superposition
- Deformation maps

Unirradiated Constitutive Behavior

- Work on both RAFMS (Spatig et al.) and V-4Cr-4Ti (Dohahue et al.) based on:
  - » Decomposition of flow stress into yield stress and strain hardening terms
  - » Defining yield stress and strain hardening terms consistent with dislocation mechanics models
  - » Calibrating terms with tensile data obtained over wide range of temperatures and strain rates

Unirradiated Flow Stress

- Unirradiated flow stress decomposed as

$$\sigma_{fl}(T,\varepsilon',\varepsilon) = \sigma_y(T,\varepsilon') + \sigma_\varepsilon(T,\varepsilon',\varepsilon)$$

- The yield stress can be decomposed as

$$\sigma_y(T,\varepsilon') = \sigma_{yt}(T,\varepsilon') + \sigma_{ya}(E(T))$$

Yield Stress

- In bcc alloys, the thermally activated yield stress component is related to kink pair nucleation on screw dislocations and/or dispersed barrier strengthening

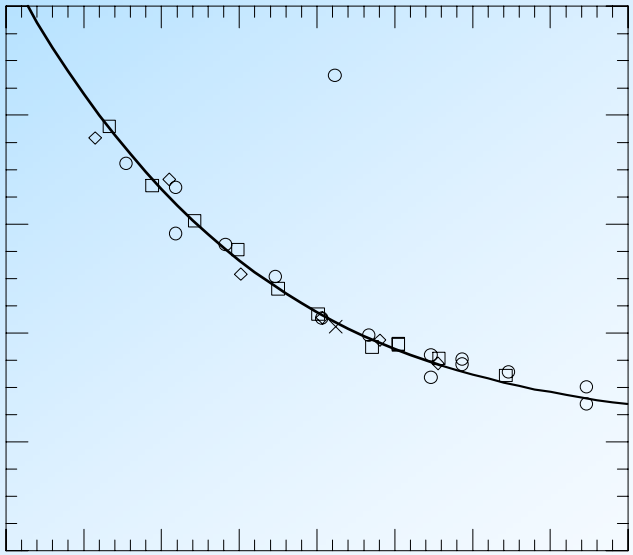
- Therefore σ_{yt} can be defined in terms of temperature compensated strain rate

$$T' = T\,[1 + C \ln (\varepsilon'_r/\varepsilon')]$$

Yield Stress

- The form of the fit is consistent with thermally activated kink formation, and can be modified for more than on thermally activated mechanism

$$\sigma_{yt}(T') = \sigma_t[1-(T'/T_c]^{1/g1}]^{g2}$$



Strain Hardening

- The strain hardening components have been found to fit a Voce-type equation, based on the generation, storage, and recovery of dislocations

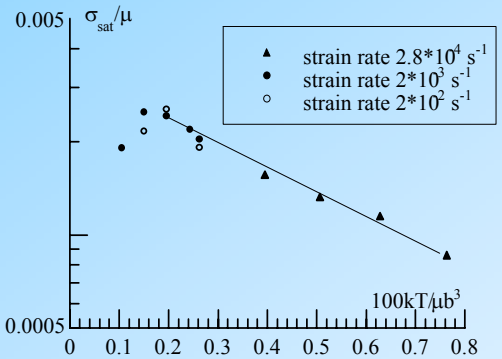
$$\theta_p = d\sigma_{pl}/d\varepsilon_p = K_1(\varepsilon',T) - K_2(\varepsilon',T)\,(\sigma-\sigma_{0.1})$$

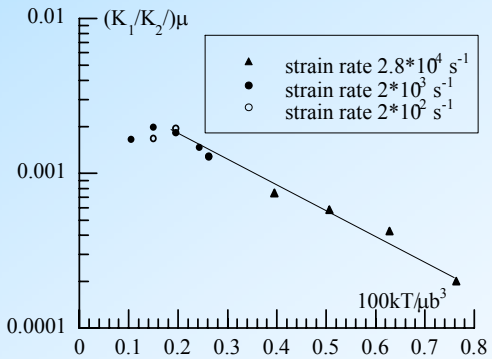
$$\sigma_\varepsilon(T,\varepsilon',\varepsilon\,) = \sigma_{sat} - K_1/K_2 \exp[-K_2\,(\varepsilon_p - .01)]$$

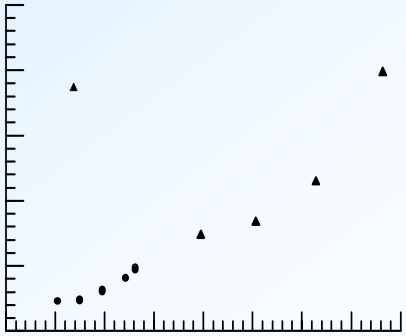
- K_1 can be related to the mean free path for dislocation glide (cell size) and K_2 to dislocation density

Strain Hardening

- The parameters σ_{sat}, K_1/K_2 and K_2 can be determined from fits to tensile data

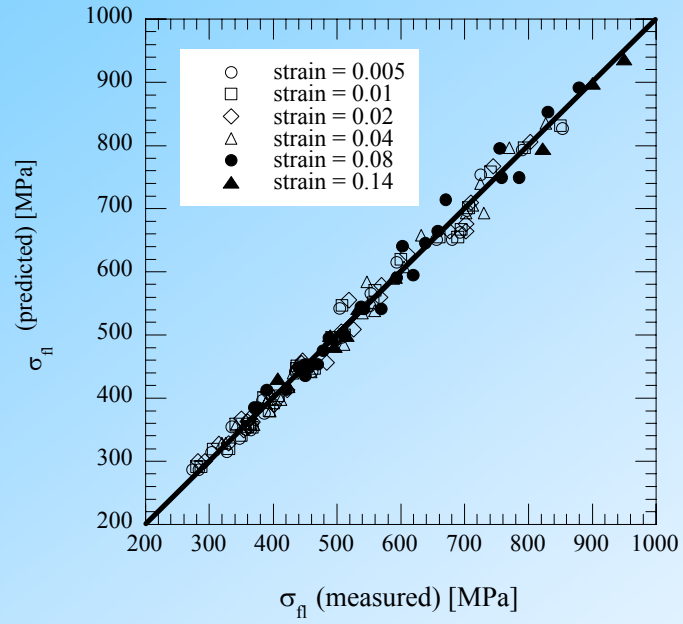




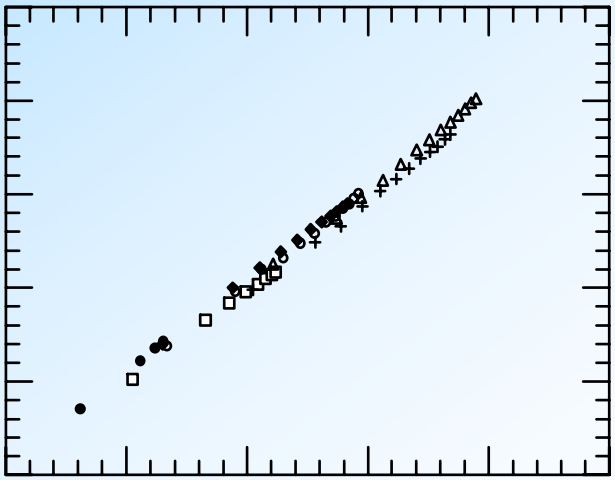


Constitutive Law

- The dislocation-mechanics based, empirically calibrated flow laws fit a wide range of data -- provide a mechanistic framework for $\sigma_{fl}(T,\varepsilon',\varepsilon)$



V-4Cr-4Ti-- Donahue et al



F82H -- Spatig et al

Constitutive Laws

- While this has been a successful approach to date, it has only been examined in a limited number of materials
- The microstructural connection, while implied, has not been fully explored and demonstrated
- The role of stress state and dilation (e.g., growing plasticity-induced void population) is unexplored

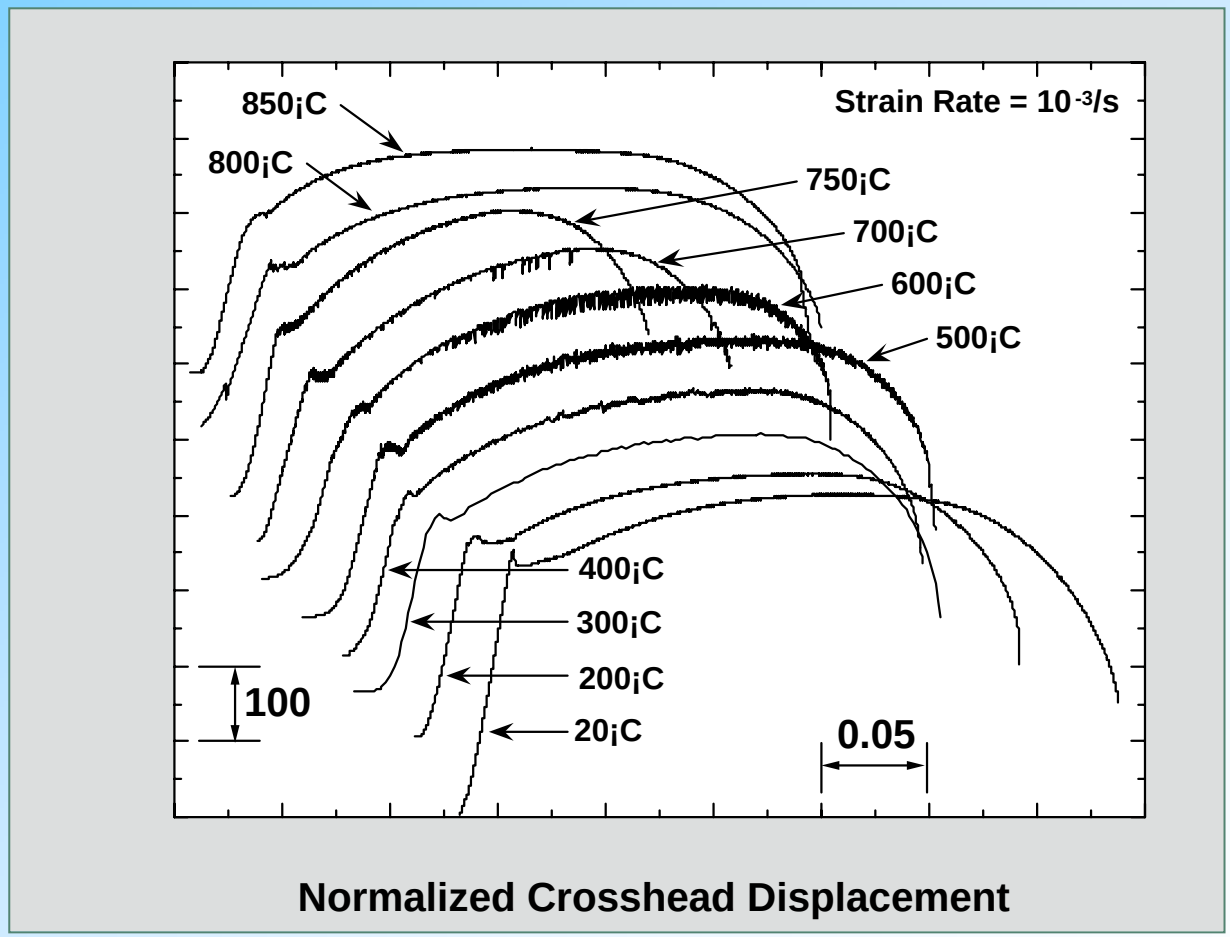
Dynamic Strain Aging In Vanadium

- At temperatures where interstitial solutes are mobile, serrated yielding occurs in the Lüders extension and jerky flow (Portevin-Le Chatelier) occurs in the strain-hardening regime due to DSA.
- The DSA regime is bounded by certain values of temperature and strain rate and is characterized by negative strain rate sensitivity (SRS) parameter:

$$m = \frac{1}{\sigma} \frac{\delta\sigma}{\delta \ln \dot{\varepsilon}} \Big|_{\varepsilon, T}$$

Load-Elongation Curves For Annealed V-4Cr-4Ti

- maximum in strain-rate sensitivity occurs at 600°C in V-4Cr-4Ti



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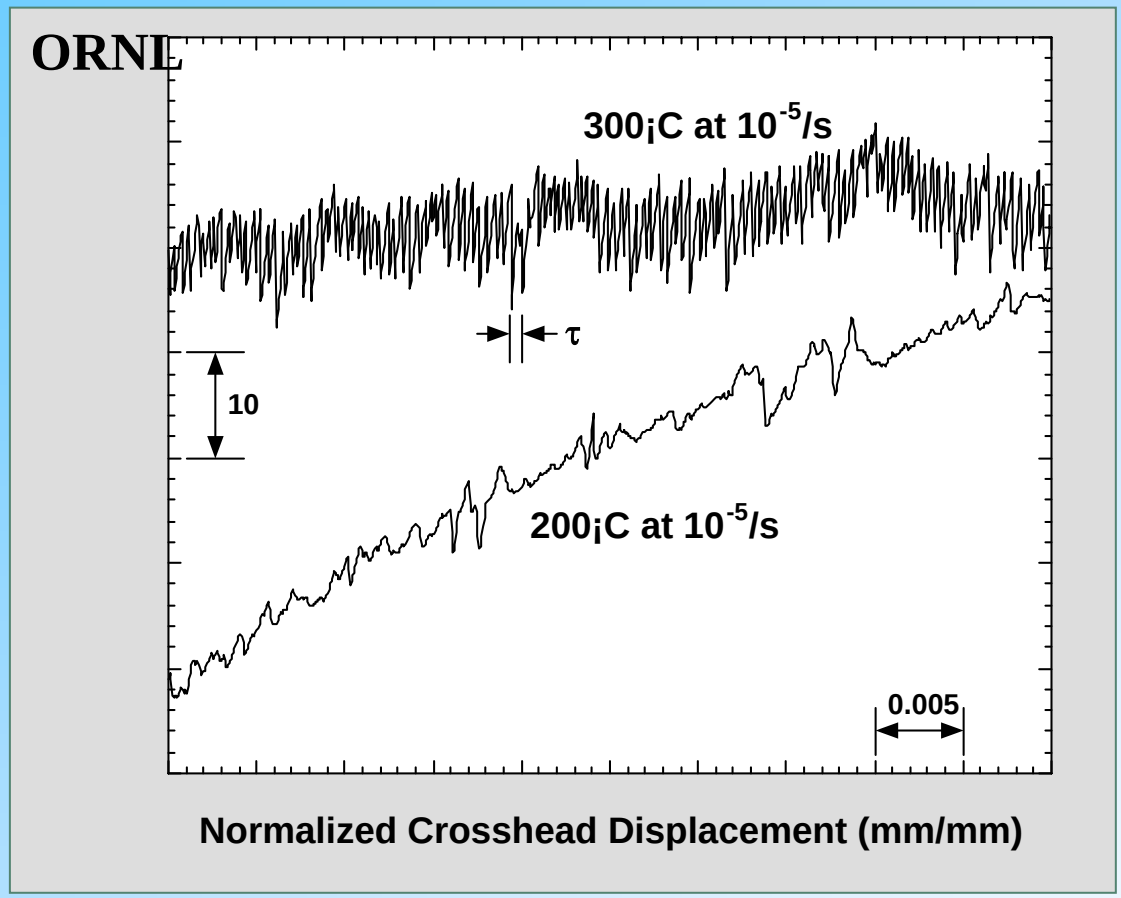
Magnified View of Serrated and Jerky Flow Behavior in Vanadium



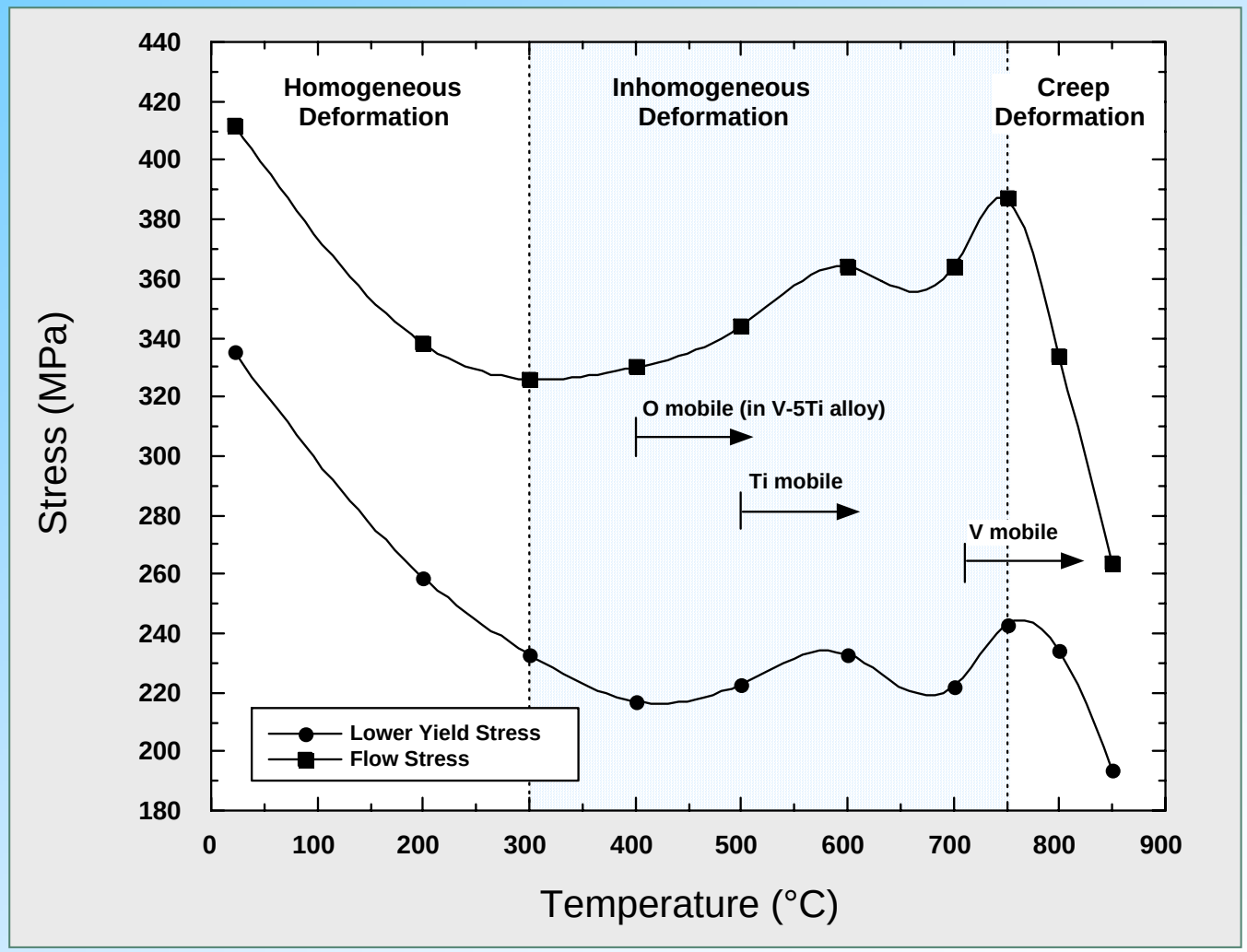
- **Estimate time for diffusion of interstitials**
  - **segregate to immobile and mobile dislocations**
  - **identify elements responsible for DSA**
- **Calculate average time between minima (τ)**
  - **300°C and 10^{-5}/s**

    τ = ~37.5s
  - **200°C and 10^{-5}/s**

    τ = ~129s

- Diffusivity calculations show:
  - Carbon and oxygen are primarily responsible for DSA effect below 300°C
  - Nitrogen has similar mobility at a higher temperature of 400°C

Temperature Dependence of σ_Y and σ_f For A Strain Rate of 10^{-3} s^{-1}



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Interstitial Impurities

- Interplay between interstitials and radiation damage remains to be fully understood
  - » Loop and point defect trapping
  - » Precipitation of Ti-C-O-N
  - » Effect on DSA
- DSA could be used as a tool to track interstitial behavior as a function of irradiation

Hardening Models

- Most irradiation hardening models assume a barrier strengthening approach:

$$\sigma_{yirr}(T,\varepsilon') = \sigma_{yt}(T,\varepsilon') + \sigma_{ya}(E(T)) + \Delta\sigma_{yirr}$$

$$\Delta\sigma_{yirr} = M\alpha\mu b/l = M\alpha\mu b\sqrt{Nd}$$

- Obstacle strengths, α, confounded by assumed values of M, superposition laws, defect population resolution -- little fundamental work for fusion materials of interest -- big opportunity for integrated modeling and experiment

Superposition Laws

- Little work in fusion beyond linear and rms assumptions of superposition

$$\Delta\sigma_L = \sum \Delta\sigma_i \qquad \Delta\sigma_R = \sqrt{\sum \Delta\sigma_i^2}$$

- Work based on dislocation glide simulations in the RPV community has shown that

$$\Delta\sigma_{irr} = S\,\Delta\sigma_L + (1-S)\,\Delta\sigma_R$$

Where (rms) $0 < S < 1$ (linear)

Odette et. al

Superposition -- cont'd

- While the functional dependence of the superposition parameter S has been worked out for two-defect populations characteristic of RPV steels, there is little work on microstructures and multiple defect populations pertinent to fusion materials and conditions

- Hence a significant opportunity exists to integrate modeling and experiment to address this issue.

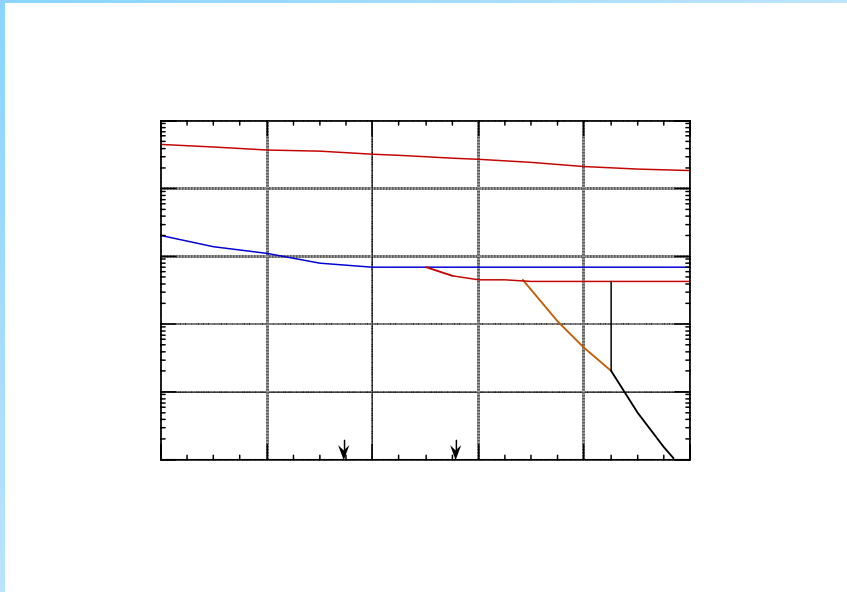
Post Yield Deformation

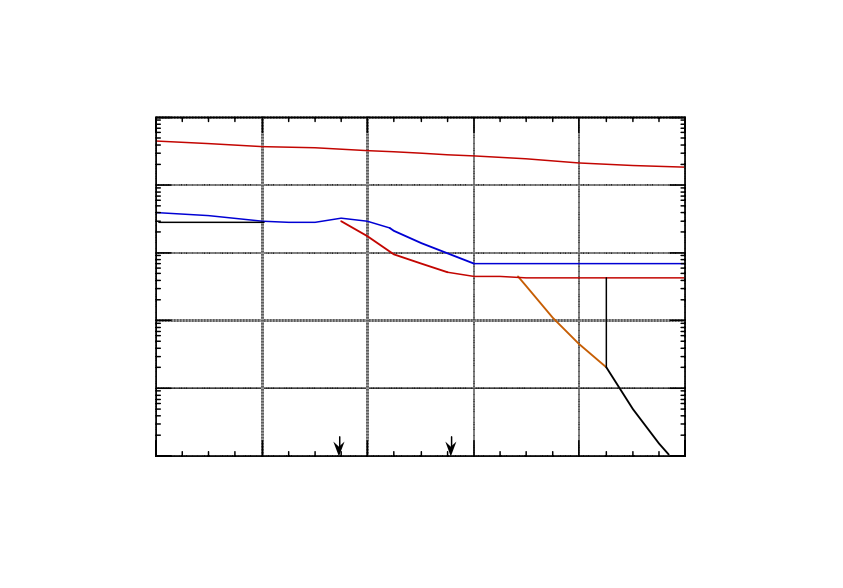
- Only recent work on modeling post-yield deformation and linking macroscopic observables to underlying constitutive laws (see later talk by Odette) -- a fertile area for improved understanding

- Effects of stress state (pure shear, multiaxial stresses,…) on yield and post-yield deformation also requires new experimental methods and strong links to modeling (FEA)

Deformation Maps

- Preliminary work begun to develop deformation (and fracture) maps for irradiated materials





Zinkle

Deformation/Fracture Maps -- cont'd

- Substantial opportunity to develop these for fusion materials systems of interest
- Outstanding questions on how to incorporate:
  - » Creep-swelling interactions
  - » Flow instabilities, work softening
  - » Fracture mode transition in bcc alloys
  - » Shear decohesion