Neutron Diffraction and Micromechanics Studies of the Fatigue Crack Deformation Behavior

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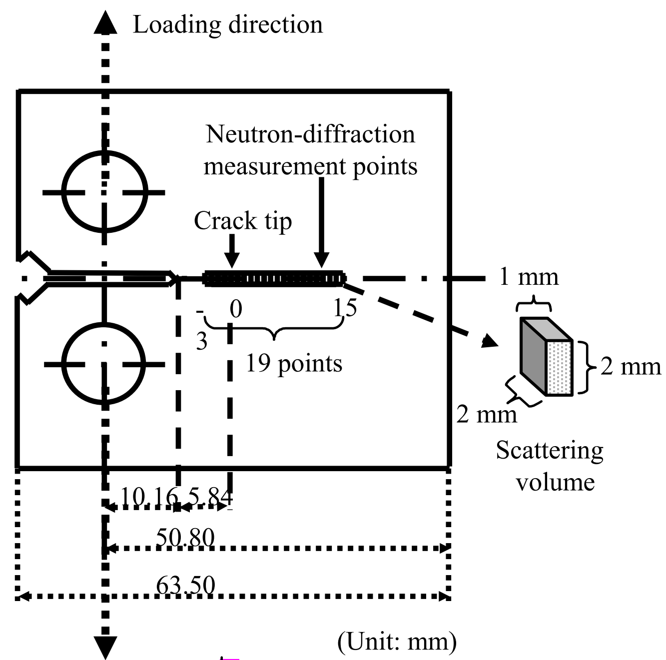
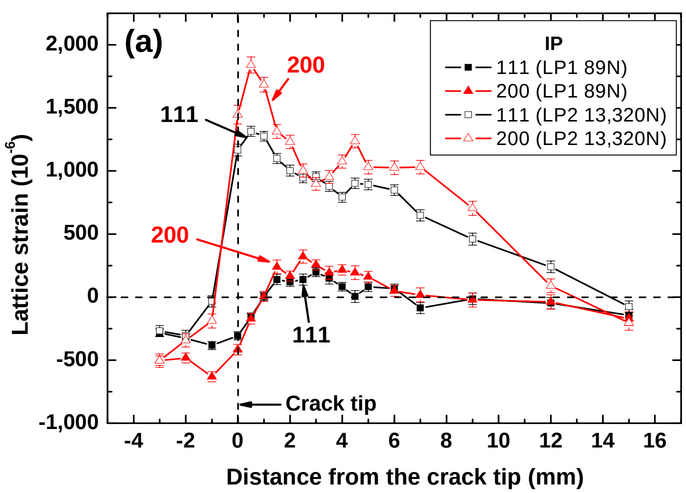
1/21-1/21/2010, VULCAN Workshop at ORNL

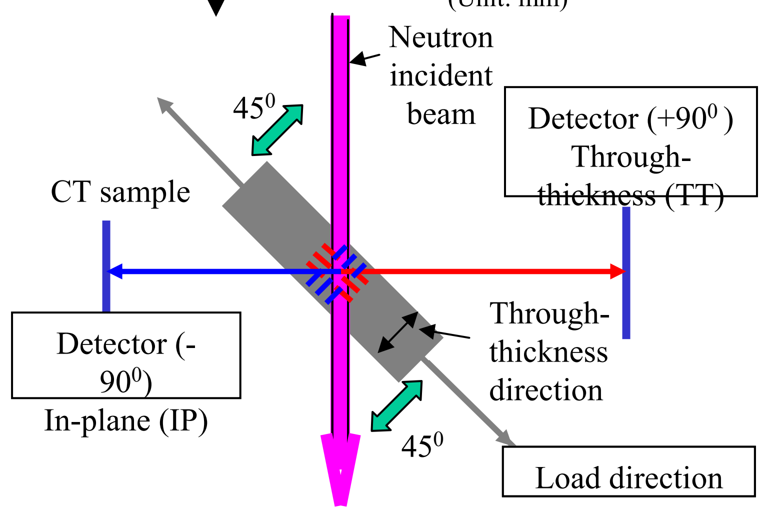
Work supported by NSF and UT-ORNL Joint Institute for Neutron Sciences

Neutron Strain Measurements of Fatigue Crack

- A standard compact tension specimen was tested at the Los Alamos Neutron Science Center (LANSCE)
- A representative result is shown for a HASTELLOY® C-2000® Alloy (58wt.%Ni-23wt.%Cr-16wt.%Mo, single-phase FCC, E=207GPa, Y=393MPa, grain size=90 ± 20 μm)
- Lattice strain distribution near the crack tip at P_{max} and P_{min}



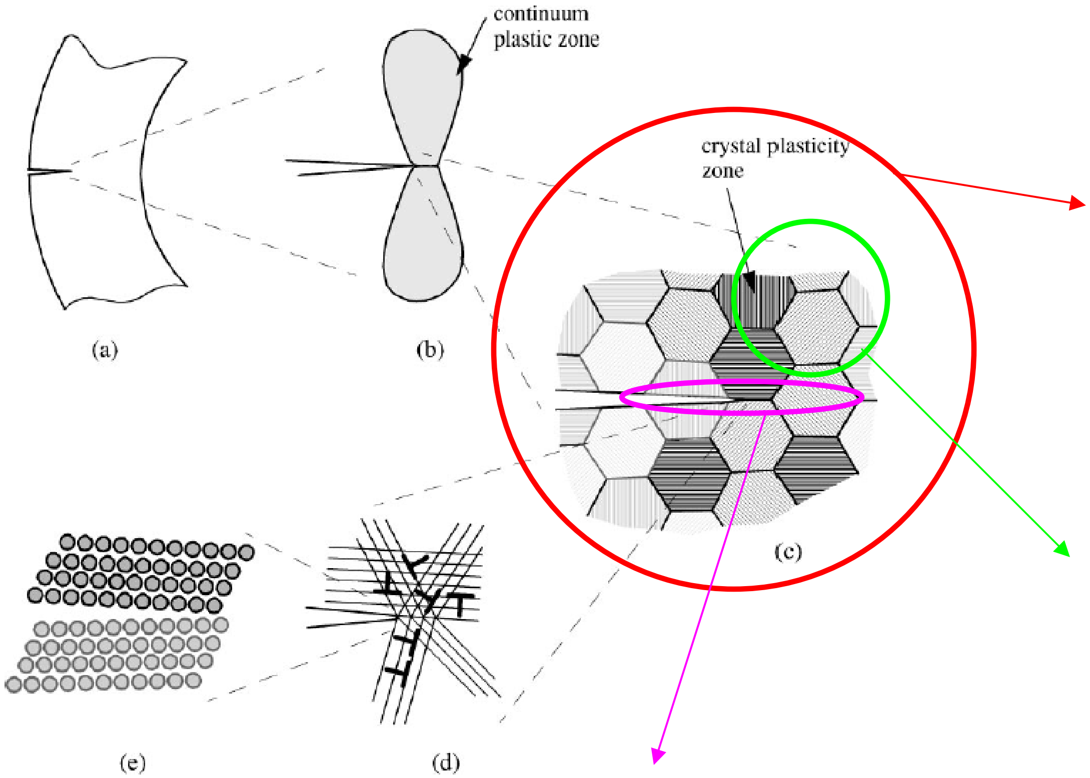




Barabash, Gao, et al., Phil. Mag. Lett. 88, 553-565 (2008)
S.Y. Lee, PhD thesis, University of Tennessee (2009)

A Multiscale View of the Crack Tip Plasticity

- Using computer simulations and neutron strain measurements, we aim to quantify the dependence of surrounding plasticity and fatigue growth behavior on material properties, load pattern, microstructure, etc
- A numerical tractable formulation is by the decoupling of scales = continuum plasticity simulations of fatigue behavior + crystal plasticity simulations of microstructure and lattice strains



- Computational modeling of elastic-plastic fracture mechanics
- Use continuum plasticity models without a reference to the material microstructure

- Lattice strain measured over many grains by neutron diffraction
- Comparison between models and experiments can enrich our understanding of polycrystal plasticity

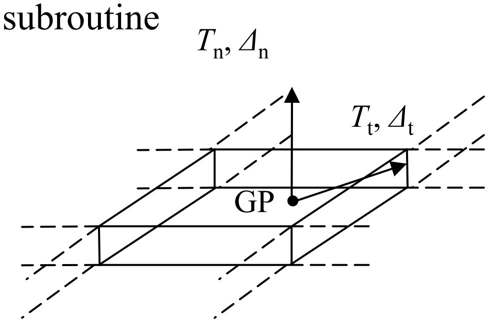
- An irreversible, hysteretic cohesive interface model to allow fatigue crack growth
- Plastic wake can be simulated

Figure as courtesy of Needleman (Brown Univ.)

Hysteretic, Irreversible Cohesive Zone Model

- Cohesive interface model prescribes a set of traction-separation constitutive law for weak interfaces
- Implemented in ABAQUS User-defined ELement (UEL) subroutine

$$\int_V \sigma_{ij}\delta\varepsilon_{ij}dV + \int_{\Gamma_{int}} T_\alpha \delta\Delta_\alpha dA = \int_{\Gamma_{ext}} t_i^* \delta u_i dA$$



GP: Gaussian point in the cohesive element

- An irreversible, hysteretic formulation will introduce a damage mechanism which allows the formation of a fatigue crack

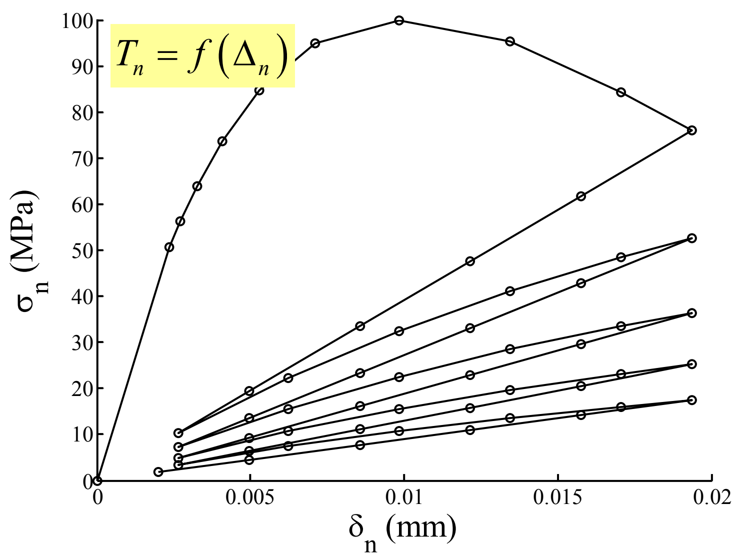
$$\dot{T}_n = \begin{cases} K^- \dot{\Delta}_n, & \dot{\Delta}_n < 0 \\ K^+ \dot{\Delta}_n, & \dot{\Delta}_n > 0 \end{cases}$$

unloading stiffness

$$K^- = \frac{T_n^{unload}}{\Delta_n^{unload}}$$

reloading stiffness

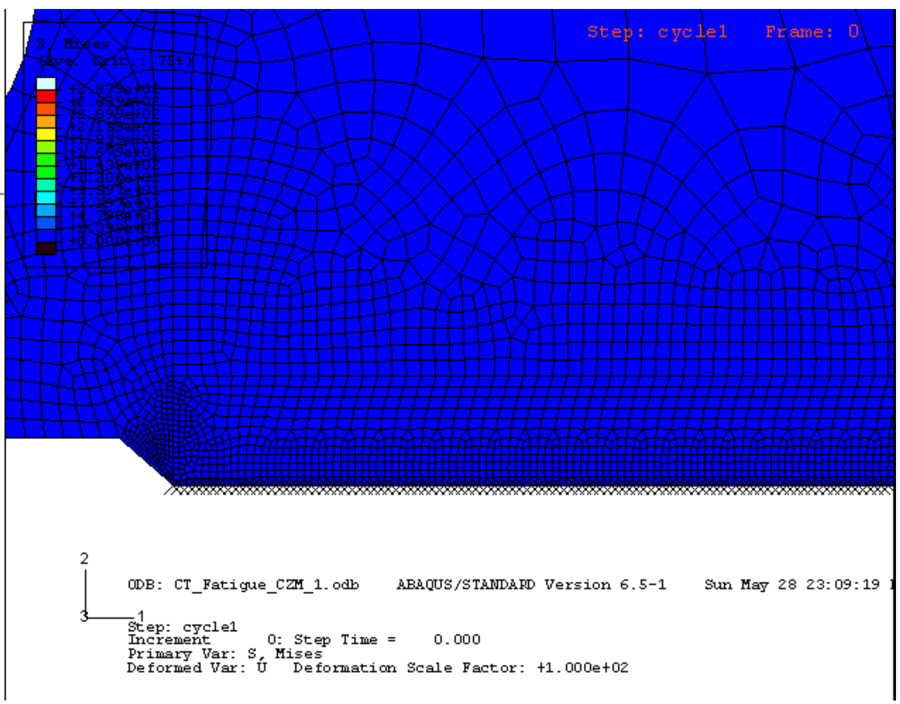
$$\dot{K}^+ = \begin{cases} -K^+ \dfrac{\dot{\Delta}_n}{\delta_f}, & \dot{\Delta}_n > 0 \\ \left(K^+ - K^-\right)\dfrac{\dot{\Delta}_n}{\delta_a}, & \dot{\Delta}_n < 0 \end{cases}$$



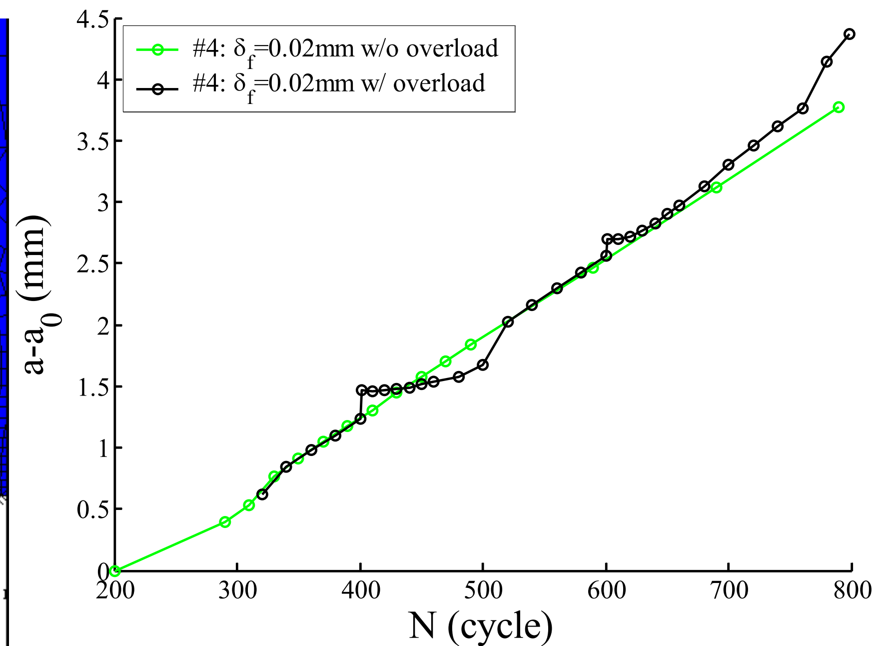
Nguyen et al., Int. J. Fract. 110, 351-369 (2001)
Gao and Bower, Modelling Simul. Mater. Sci. Eng. 12, 453-463 (2004)
-- free download of ABAQUS UMAT template at http://web.utk.edu/~ygao7/publication.htm

Fatigue Crack Growth and Overload Effects

- The *phenomenological* cohesive interface model can faithfully reproduce a steady fatigue crack if
  - A plastic wake should emerge and be larger than the plastic zone size
  - Crack increment is much smaller than the plastic zone and crack bridging zone
  - Crack bridging zone is smaller than the plastic zone
- Although a smooth crack growth is predicted, d*a*/dN is far different from experiments
- Preliminary studies on overload effects show crack growth retardation



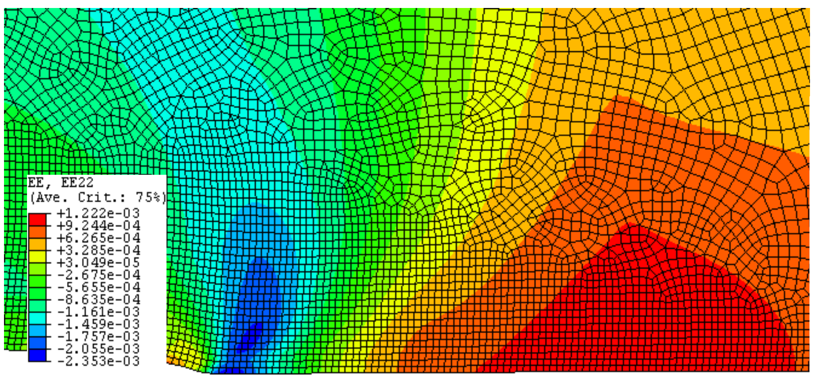
Example #1: Mises stress for δ_f=0.004mm

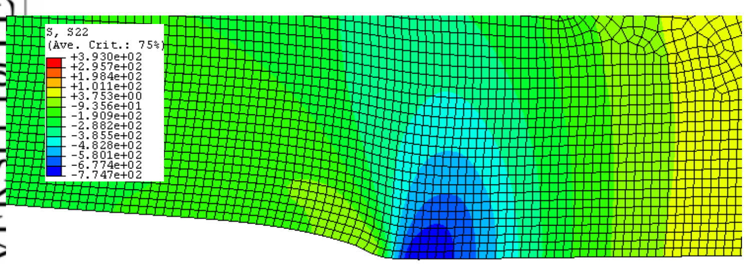


σ_{max} (MPa)	δ_n (μm)	δ_a/δ_n	δ_f/δ_n	E (GPa)	ν	σ_{max} (MPa)
800	1	0.4	4	210	0.3	288

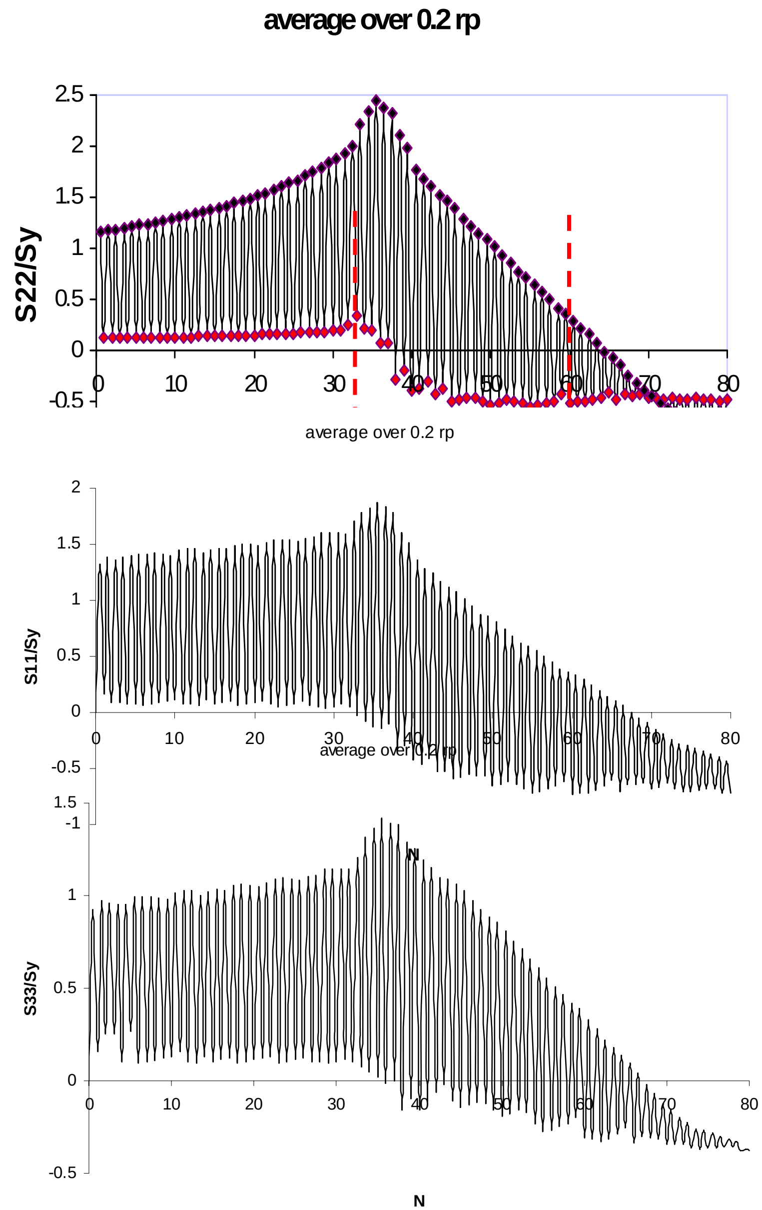
Experimental Comparisons – HASTELLOY® C-2000® Alloy

- ε_{22} (as obtained from lattice strains) will exhibit a compressive-to-tensile transition as we traverse from the plastic wake to crack front
- However, in order to obtain ε_{hkl} distribution, we need to use stress history as inputs for a polycrystal plastic simulation





$r_p/3$



Finite Deformation and Crystal Plasticity

- Multiplicative decomposition

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \qquad F_{ij} = \frac{\partial x_i}{\partial X_j} = F^e_{ik} F^p_{kj}$$

- Velocity gradient

$$\dot{\mathbf{F}}^p \mathbf{F}^{p-1} = \sum_\alpha \dot{\gamma}^{(\alpha)} \mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)}$$

- Elasticity

$$\mathbf{T} = \mathbb{C} : \mathbf{E}^e \qquad \mathbf{T} = J\mathbf{F}^{e-1} \boldsymbol{\sigma} \mathbf{F}^{e-T}$$

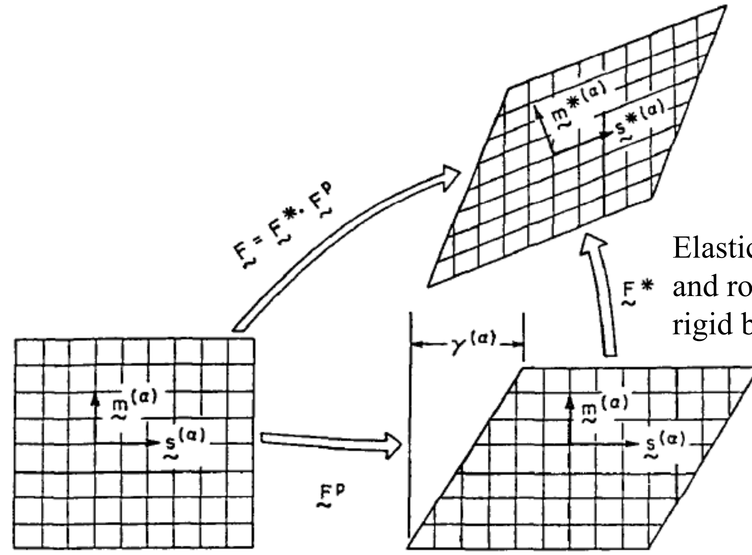
$$\mathbf{E}^e = \frac{1}{2}\left(\mathbf{F}^{eT}\mathbf{F}^e - \mathbf{I}\right)$$

- Flow rule

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{\tau^\alpha}{g^\alpha}\right)^{1/m}$$

τ^α is the resolved shear stress of α slip system $\quad \tau^\alpha = m^\alpha_i F^{e-1}_{ij} J \sigma_{jk} F^e_{kl} s^\alpha_l$

g^α is shear strength of α slip system



Elastic stretching and rotation, and rigid body motion

Plastic deformation due to crystalline slips

- Hardening law

$$\dot{g}^\alpha = \sum_\beta h_{\alpha\beta} \left|\dot{\gamma}^\beta\right|$$

hardening moduli

$$h(\gamma) = h_0 \operatorname{sech}^2 \left|\frac{h_0 \gamma}{\tau_s - \tau_0}\right|$$

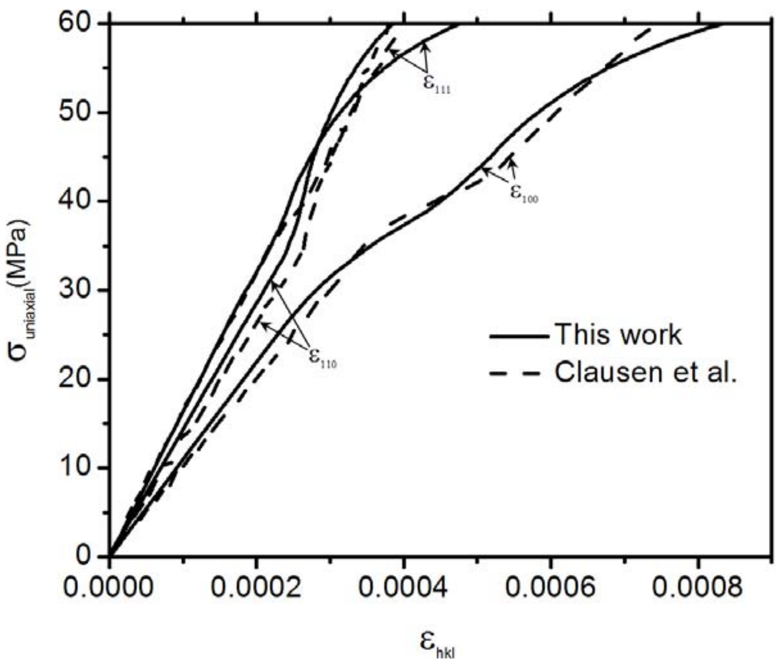
latent hardening coefficient: q

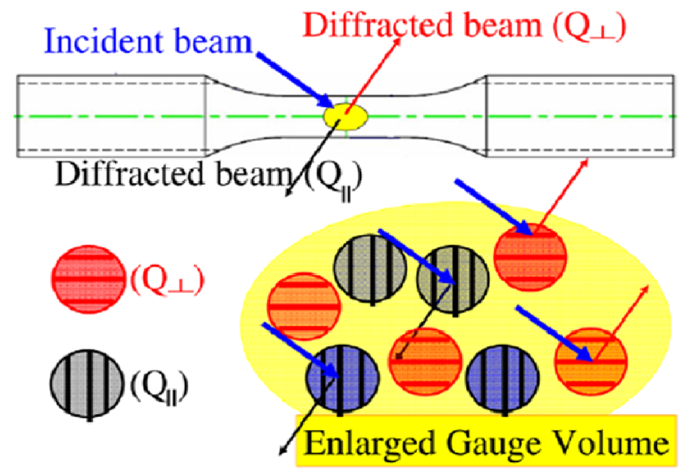
$$h_{\alpha\beta} = h(\gamma)\left[q + (1-q)\delta_{\alpha\beta}\right]$$

Peirce, Asaro, Needleman, Acta Met. 1982
Bower and Wininger, J. Mech. Phys. Solids 2004

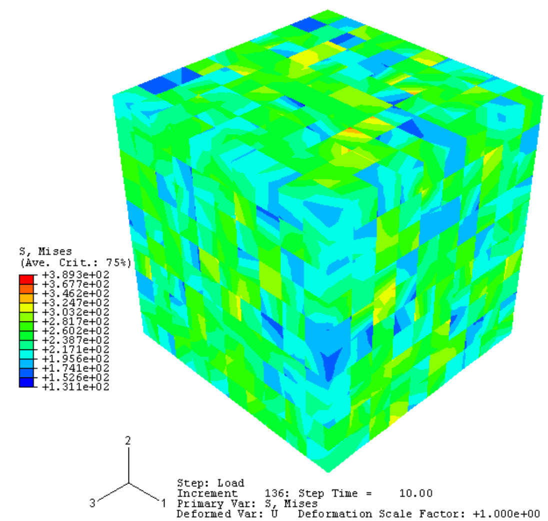
Lattice Strain Evolution

- Finite element simulations of Cu polycrystal (cubic grains, random orientations)
- Compare to the viscoplastic self-consistent (VPSC) model (Clausen et al., Acta Mat. 1998)





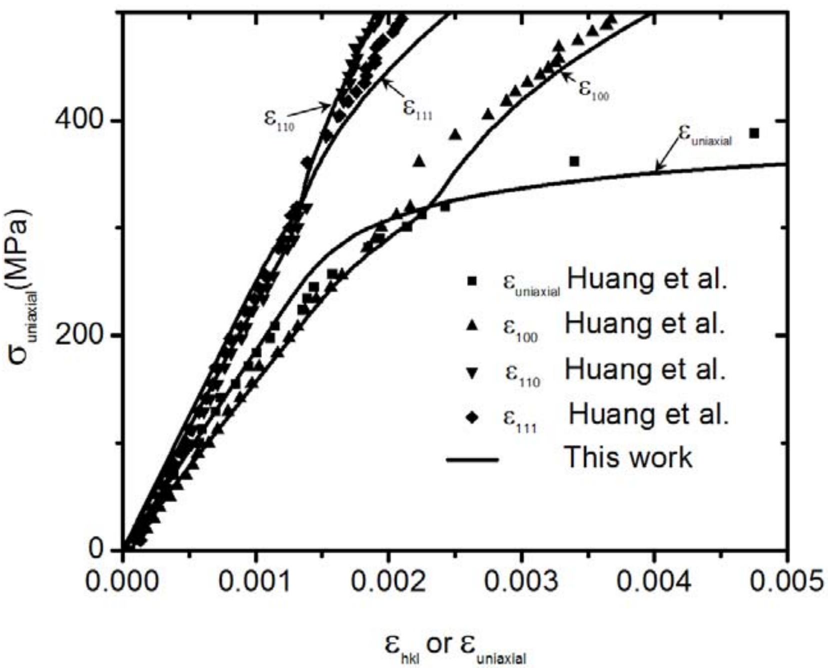
(c) Schematic grain-oriented-dependent diffraction



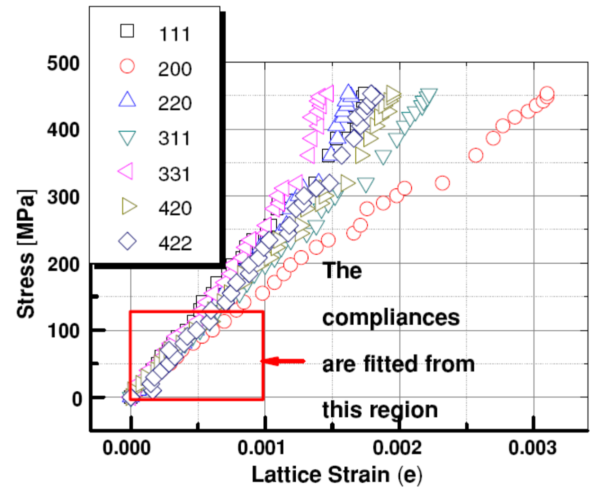
c_{11} (GPa)	c_{12} (GPa)	c_{44} (GPa)	m	h_0 (MPa)	τ_0 (MPa)	τ_s (MPa)	q
168.4	121.4	75.4	50	120	15	20	1.0

Experiments on HASTELLOY® C-22HS® Alloy

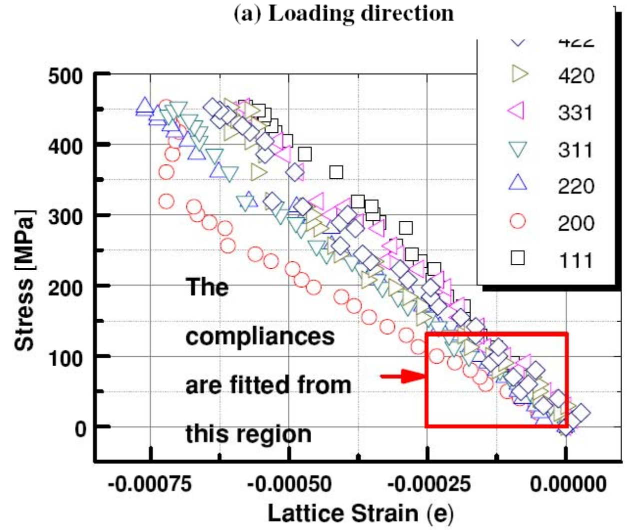
- Using elastic constants fitted from $\sigma \sim \varepsilon_{hkl}$ curves, a good agreement can be made between neutron measurements and crystal plasticity simulations



c_{11} (GPa)	c_{12} (GPa)	c_{44} (GPa)	m	h_0 (MPa)	τ_0 (MPa)	τ_s (MPa)	q
303	210	106	50	550	120	750	1.0



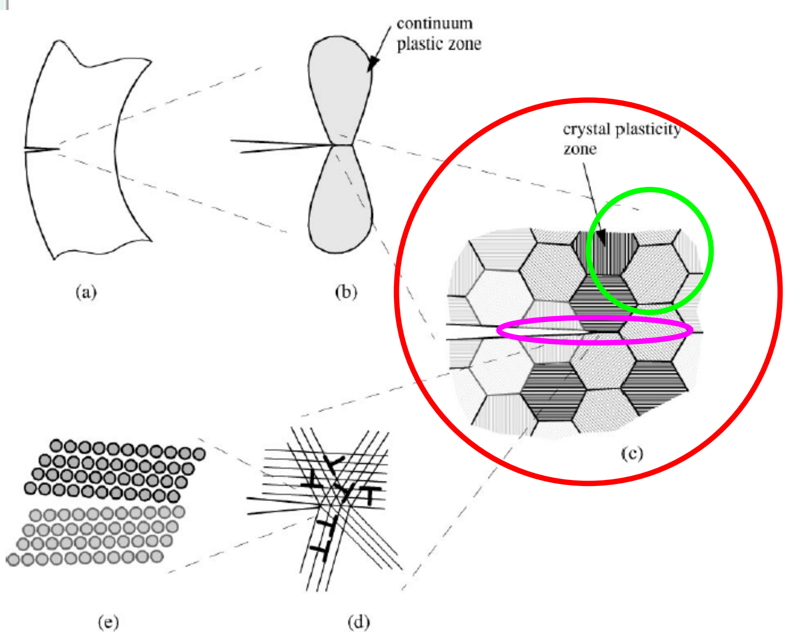
(a) Loading direction

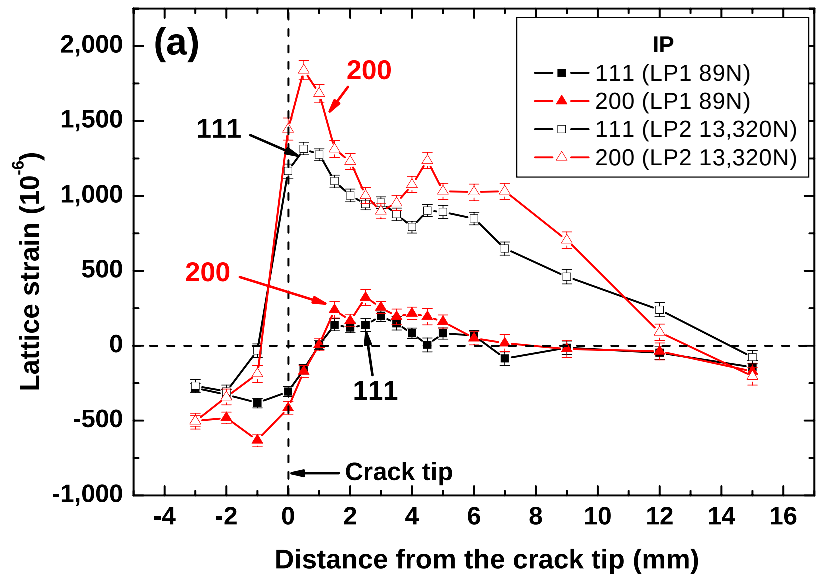


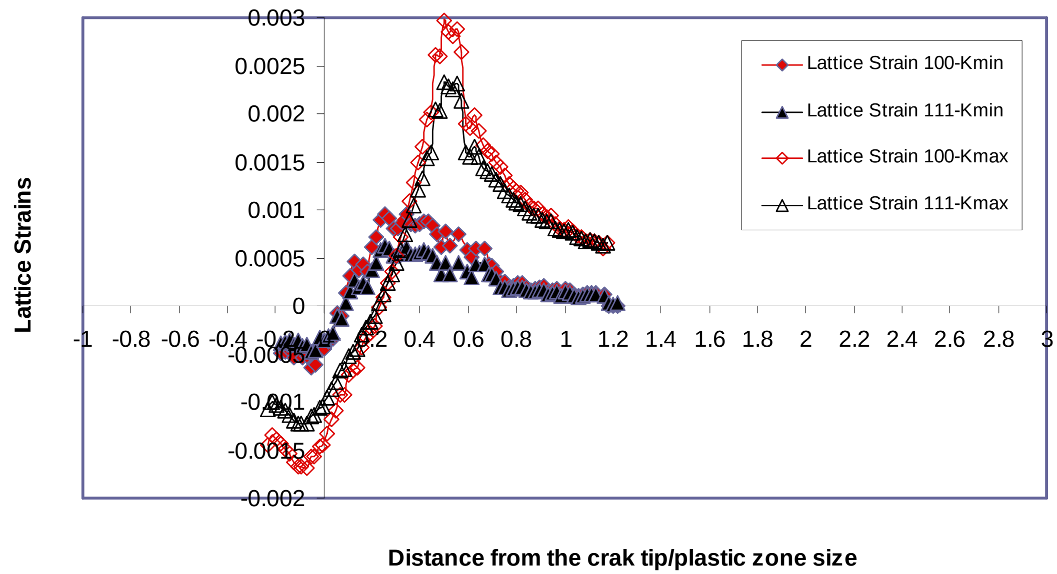
(b) Transverse direction

Huang, et al., Met Trans. A 39, 3079-3088 (2008)

Experimental Comparisons – HASTELLOY® C-2000® Alloy







Pros

- Connections between continuum residual stress analysis and lattice strain evolution

Cons

- Separation of length scales
- Not suitable for short cracks because of complicated fatigue mechanisms

Summary

- In engineering problems where scales can be separated, it appears that micromechanics model is very capable

- VULCAN as a probe on microstructural length scales motivated us to investigate the role of grain boundary deformation on lattice strain evolution