Mathematisches Forschungsinstitut Oberwolfach, Mechanics of Materials Meeting, May 5-11, 2002

Deformation Behavior Of Hadfield Steel Single And Polycrystals Due To Twinning and Slip

Huseyin Sehitoglu, D. Canadinc, Ibrahim Karaman
Department of Mechanical and Industrial Engineering, University of Illinois
Urbana, IL

Y.I. Chumlyakov
Siberian Physical Technical Institute, Tomsk, Russia

Hans J. Maier
University of Paderborn, Paderborn, Germany

National Science Foundation
Mechanics and Materials Program, Directorate of Engineering, Arlington, VI
Grants CMS 94-14525 and CMS 99-00090

Outline

Introduction to Low Stacking Fault Energy Materials- Hadfield Steel

Constriction Energy-Planarity of Slip

Experiments on Single Crystals

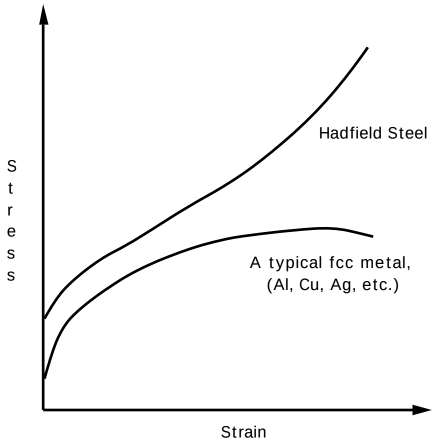
Modeling of Deformation Response

Bauschinger Experiments

Solute/Precipitate Hardening Effects

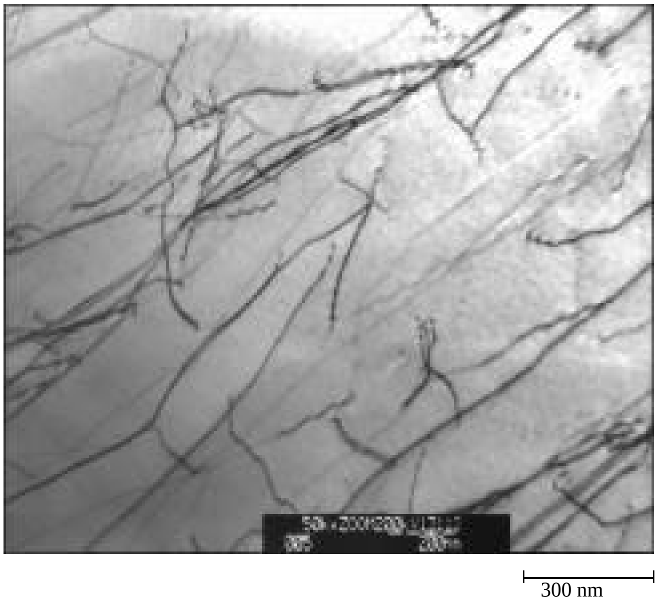
Why Study Hadfield Steel(Fe-13Mn-1C)?

- Unresolved problem of high strain hardening
- Two simultaneous deformation mechanisms (twinning and slip)
- Solid Solution Hardening
- Can we put meaningful microstructural features in a crystal plasticity framework?

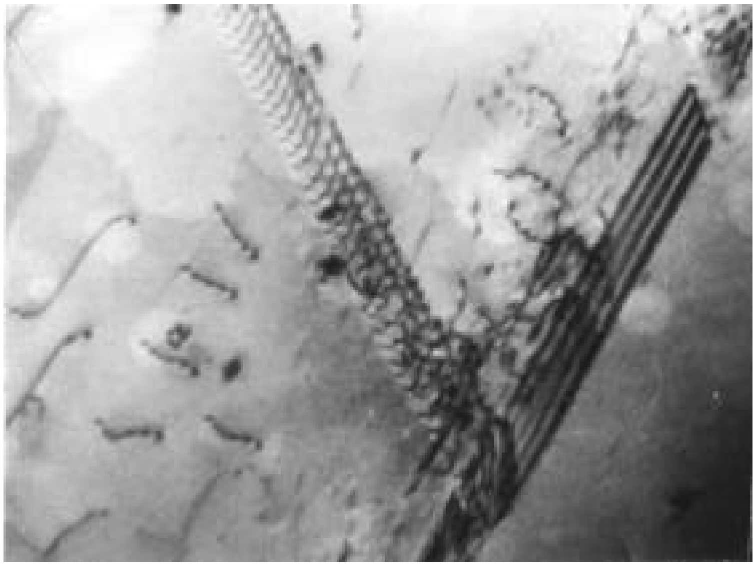


Hadfield Steel Single Crystals

Low stacking fault energy FCC(Austenitic) material (γ~23 mJ/m^2)
High interstitial atom content (5-8 at. % C)

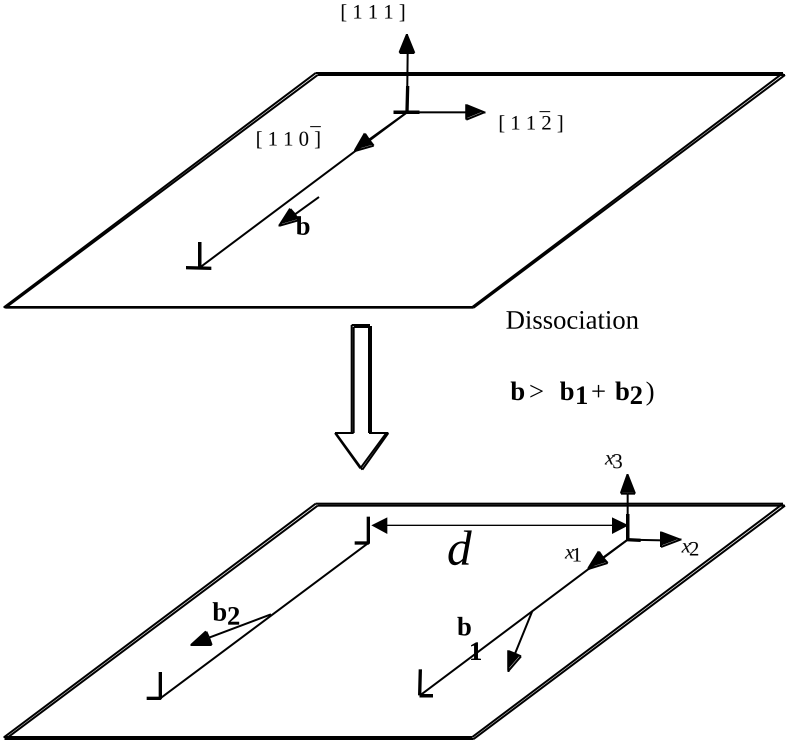


[123] Tension



[111] Tension

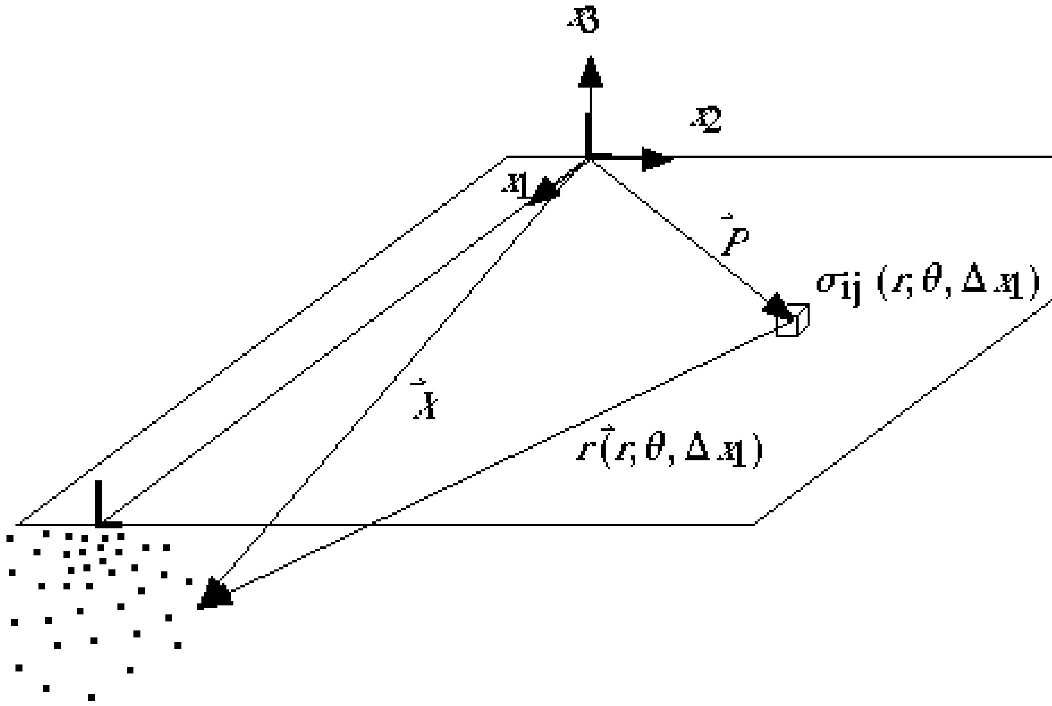
Dissociation of pure screw dislocation into two partials



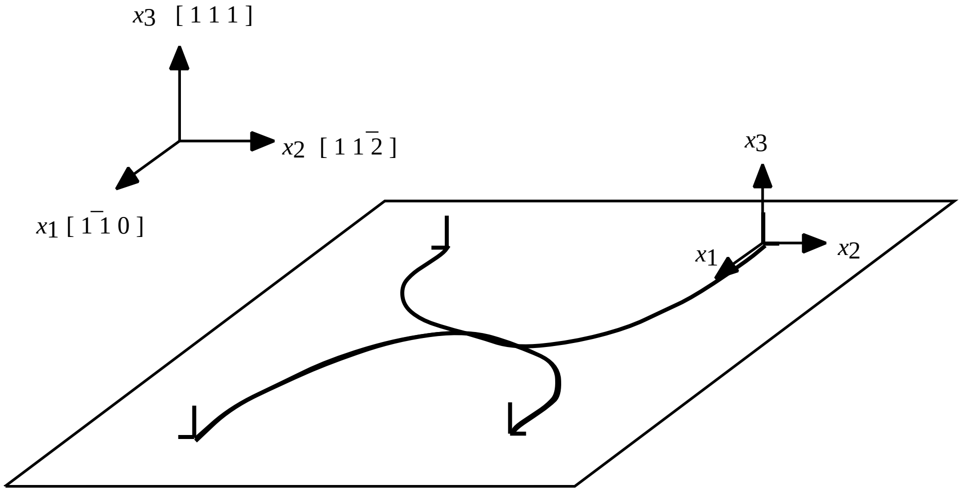
Dissociation

$\mathbf{b} > \mathbf{b_1} + \mathbf{b_2})$

Cylindrical coordinate system used for stress integration $\Delta x_1 = X_1 - P_1$



Schematic of two partials forming a constriction



Andrews, Sehitoglu, Karaman, J. Appl. Physics, 87,5,2194-2203, 2000

Equilibrium Shape of Partial Dislocations

$$\frac{A}{2x_2+d}+T^{line}\frac{d^2x_2}{dx_1{}^2}-\gamma+\sigma_{23}^{total}\left(\vec{P}\right)b_e+\sigma_{13}^{total}\left(\vec{P}\right)b_s=0$$

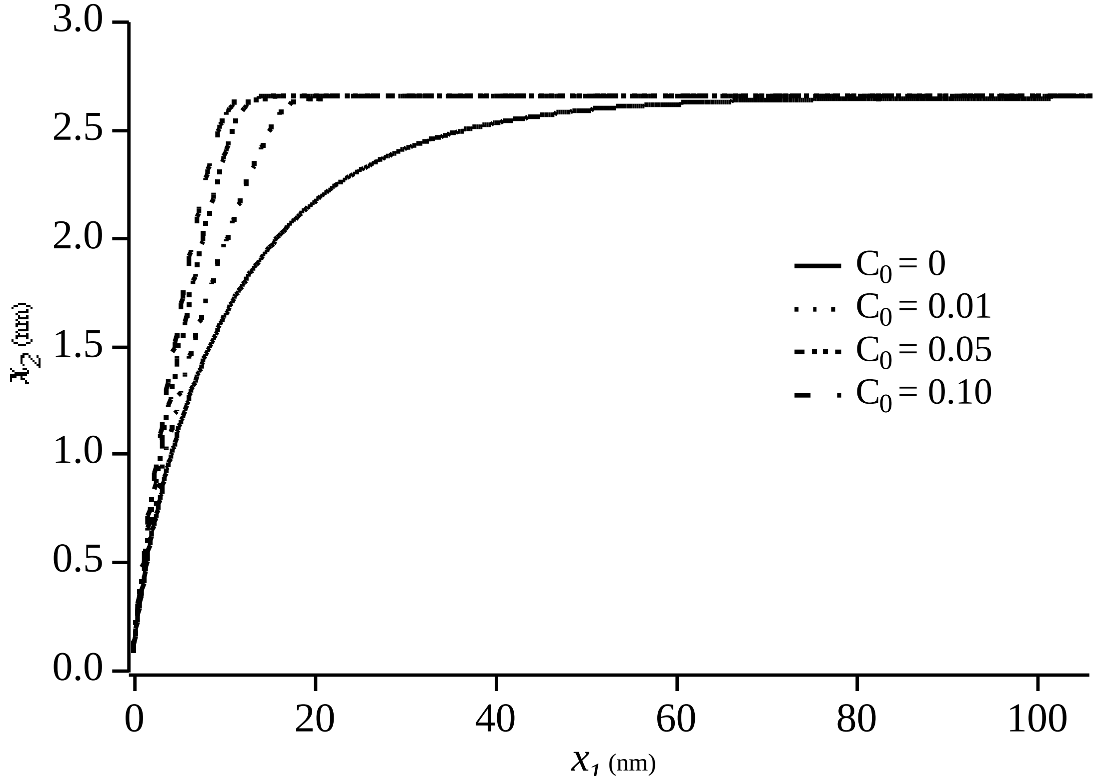
$$T^{line}=\frac{\mathbf{b_1}\mathbf{b_1}\mu}{4\pi}\ln\frac{R}{r_0}$$

$$A=\frac{\mu}{2\pi}\left(\mathbf{b_1}.\xi\right)\left(\mathbf{b}_2.\xi\right)+\frac{\mu}{2\pi(1-\nu)}\left(\mathbf{b_1}\times\xi\right)\left(\mathbf{b}_2\times\xi\right)$$

$$\sigma_{ij}^{total}\left(\vec{P}\right)=\oint_V C\left(\vec{X}\right)\sigma_{ij}\left(r,\theta,\Delta x_1\right)dV$$

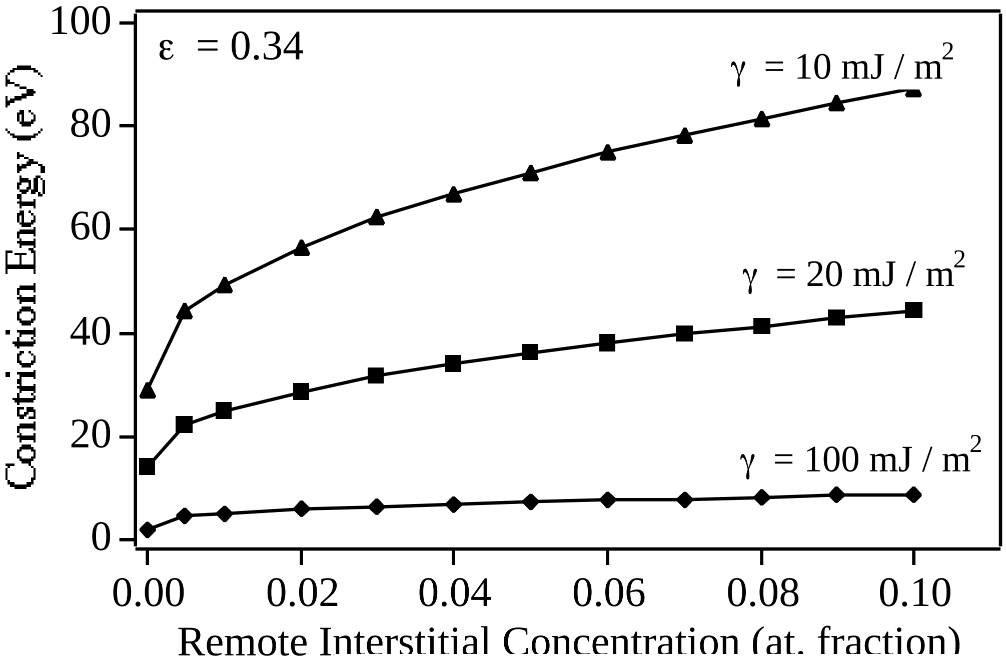
Constriction shape for several interstitial concentrations.

$\rho = 0.71$ Å. $a = 3.56$ Å. $\mu = 80$ GPa. $\varepsilon = 0.3$. $\varepsilon_G' = 0$. $\gamma = 20$ mJ / m^2.

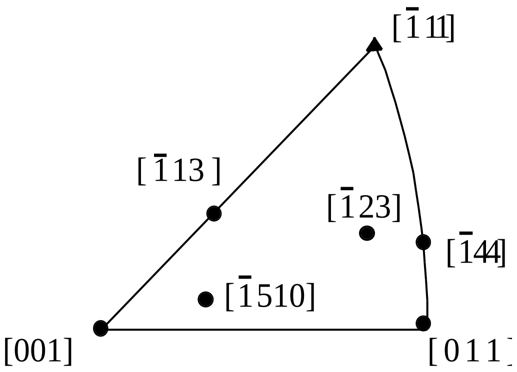


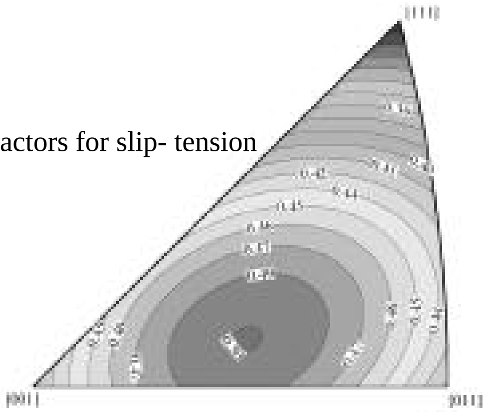
Total energy to form a constriction in an fcc metal with octahedral interstitials for various stacking fault energies.

$\rho = 0.71$ Å. $a = 3.56$ Å. $\mu = 80$ GPa. $\varepsilon_G' = 0$.

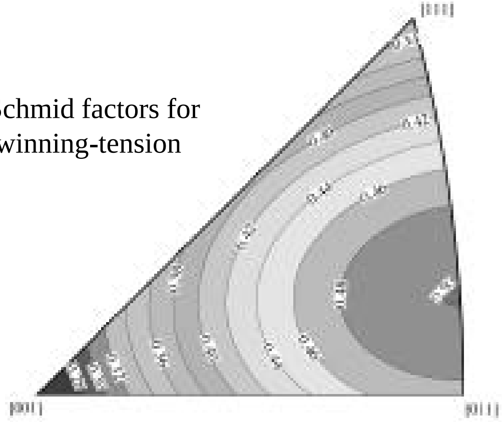


Single Crystal O





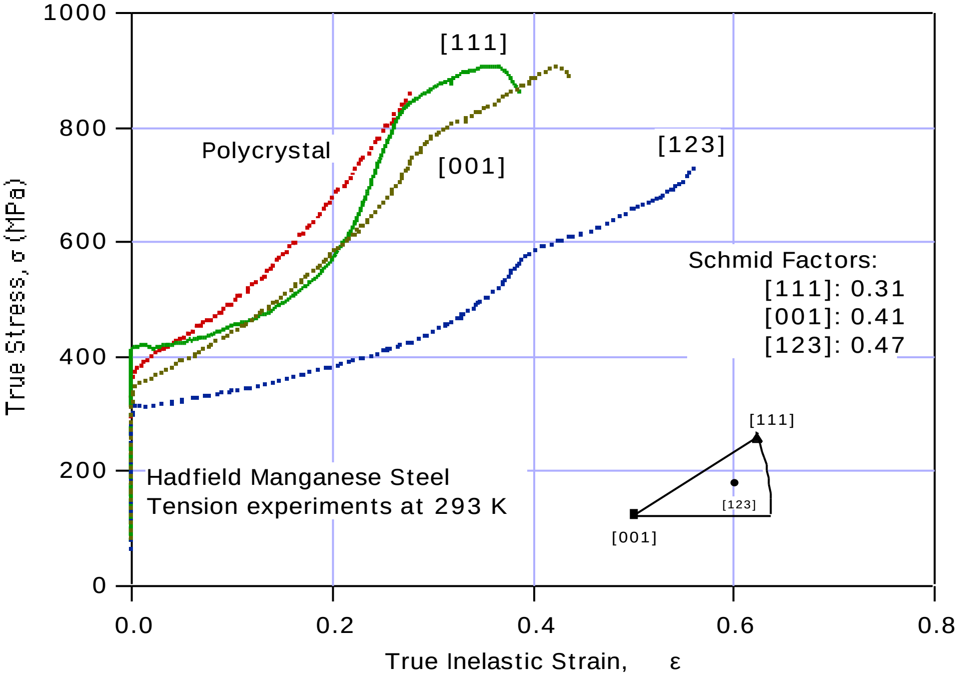
Schmid factors for slip- tension



Schmid factors for twinning-tension

- Orientations: [111], [001], [011] and [123]
- (no grain boundaries, microstructure easy to understand, modeling parameters)

Experimental Results: Room Temperature Tension Tests



CRSS:

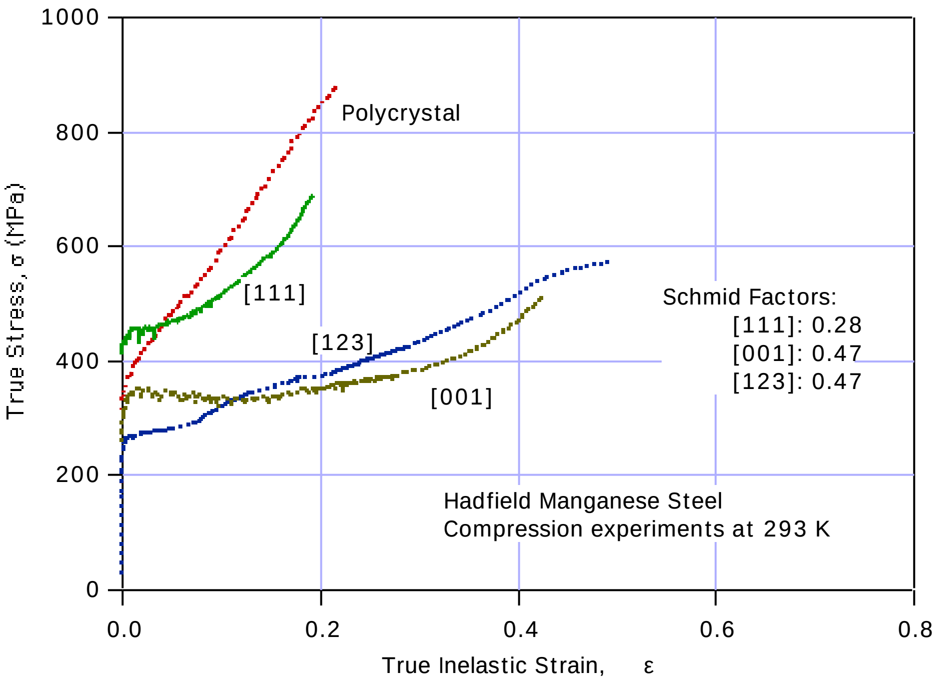
[111]= 110 MPa
[001]= 131 MPa
[123]= 138 MPa

Stage II Hardening

[111]= G/40
[001]=G/150
[123]=G/300
Typical FCC=G/300

Karaman, Sehitoglu, *et. al*, Acta Mat., 2000, Vol. 48, pp. 1345

Experimental Results: Room Temperature Compression Tests



Schmid Factors:
[111]: 0.28
[001]: 0.47
[123]: 0.47

Hadfield Manganese Steel
Compression experiments at 293 K

CRSS:

[111]= 116 MPa
[001]= 110 MPa
[123]= 119 MPa

Stage II Hardening

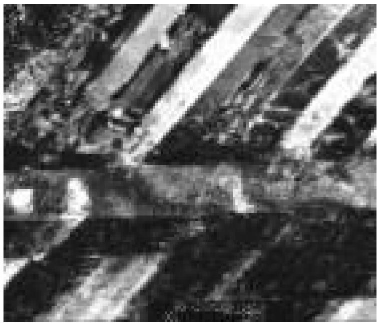
[111]= G/40
[001]=G/100
[123]=G/300
Typical FCC=G/300

[111] Orientation, Stages of Deformation TEM observations

Tension

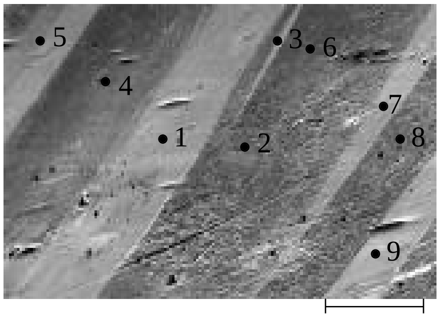
3 % Strain

25 % Strain

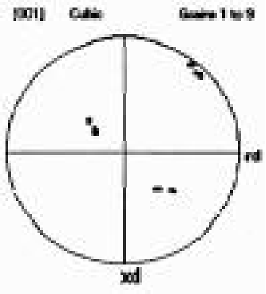


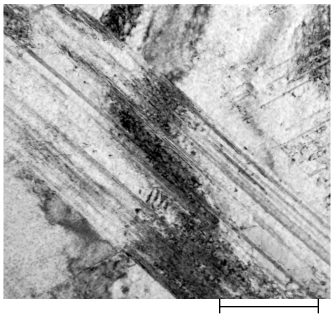
35 % Strain

Compression



3 % Strain

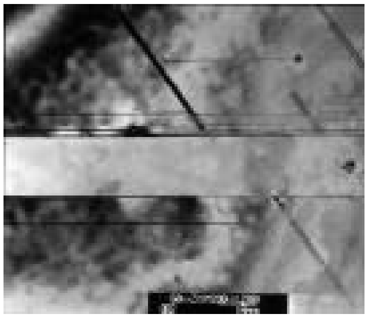




20 % Strain

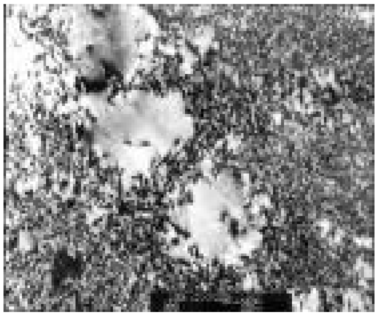
High SFE vs. Low SFE Materials Microstructure

[001] Compression



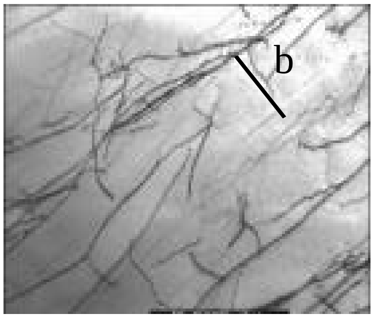
3% Strain

[001] Tension

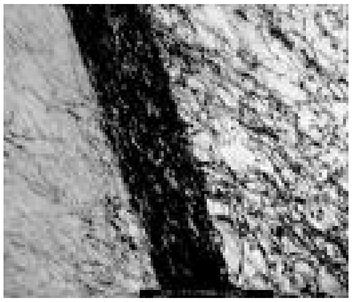


30% Strain

[123] Tension



3 % Strain



50 % Strain

Conclusions from Experimental Observations

- Governing deformation mechanism and strain hardening is orientation and stress-state dependent.
- Twinning is observed as initial deformation mechanism at room temperature. (<1% strain). Twin thickness saturates, twin volume fraction increases.
- Unusual strain hardening -> slip-twin interaction. Twin boundary-> grain boundary. How to incorporate into models?

Modeling of Stress-Strain Response
Limitations of current models

- Incorporating twinning into crystal plasticity models-> partially solved. Very few studies on low SFE fcc materials.
- Lack of physically sound hardening laws.(dislocation density, twin volume fraction, hardening due to reorientation, etc.)
- No explicit treatment of slip-twin interaction
- Single crystal parameters in the constitutive law are determined from polycrystal response.

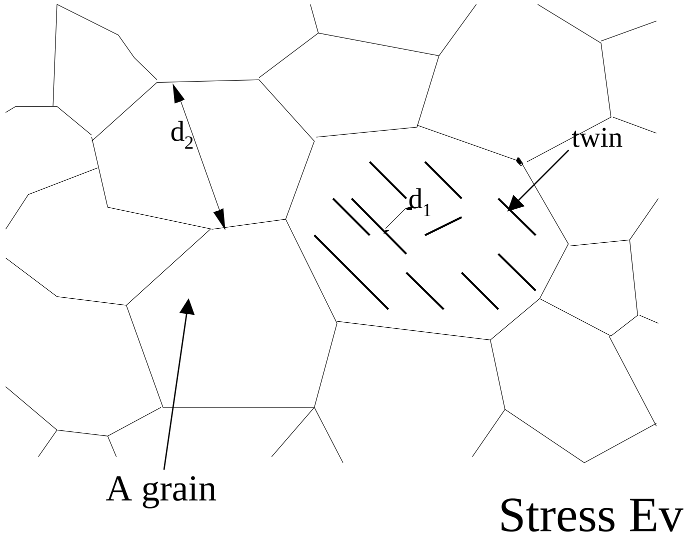
Visco-Plastic Self Consistent (VPSC) Formulation

- Kinematic equation between deformation rate and the stress(pseudo-linear form, rate dependent approach):

$$\dot{\varepsilon}_i = \left\{ \dot{\gamma}_0 \sum_{s=1}^{S} \frac{m_i^s m_j^s}{\tau_c^s} \left(\frac{m_k^s \sigma'_k}{\tau_c^s} \right)^{n-1} \right\} \sigma'_j = M_{ij}^{c(sec)} \sigma'_j$$

- A grain is an inclusion in the homogeneous effective medium.
- 1000 grain initially with same orientation (single crystals). # of grains in polycrystals ->experimental weights.
- Preferred twinning reorientation (PTR) scheme.

Incorporating the length scale into the model



$$\dot{\rho} = \sum_k \left\{ \frac{k_0}{db} + k_1\sqrt{\rho} - k_2\rho \right\} \left|\dot{\gamma}^k\right|$$

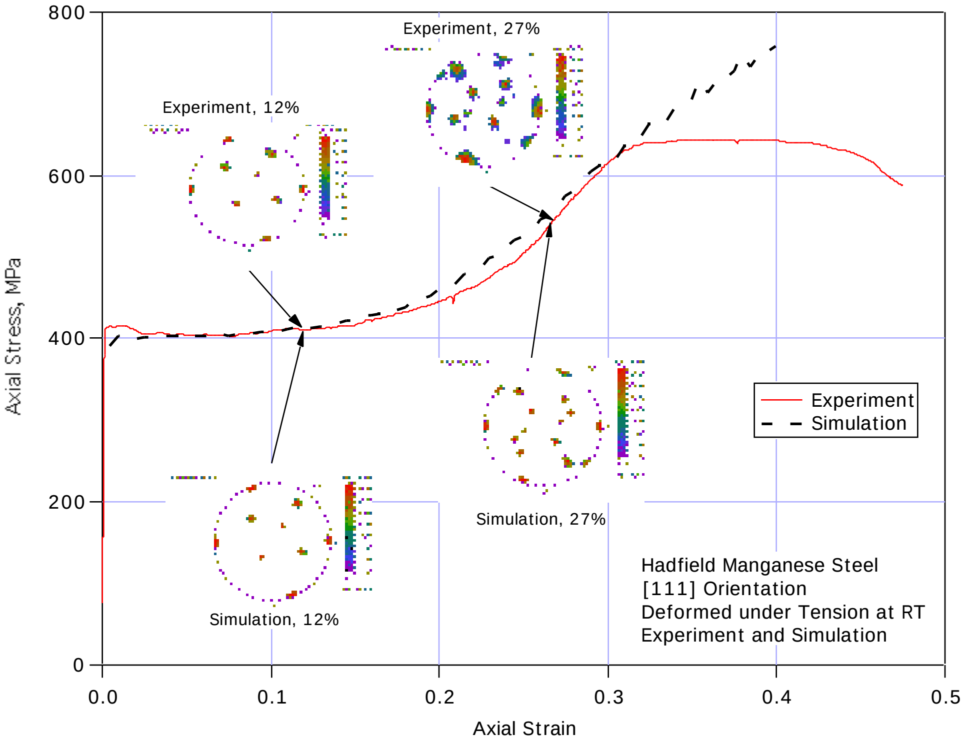
Evolution of dislocation density

d_1: Distance between twins
d_2: Average grain size

Stress Evolution

$$\dot{\hat{\tau}} = \left[\frac{\mu^2 \alpha b}{2\left(\hat{\tau} - \hat{\tau}_0\right)} \left(\frac{K_1^{\,2}}{d_1} + \frac{K_2^{\,2}}{d_2} \right) + \theta_0 \left\{ \frac{\hat{\tau}_s - \hat{\tau}}{\hat{\tau}_s - \hat{\tau}_0} \right\} + \frac{\partial \dot{\hat{\tau}}_s}{\partial \gamma} \right] \sum_k \left|\dot{\gamma}^k\right|$$

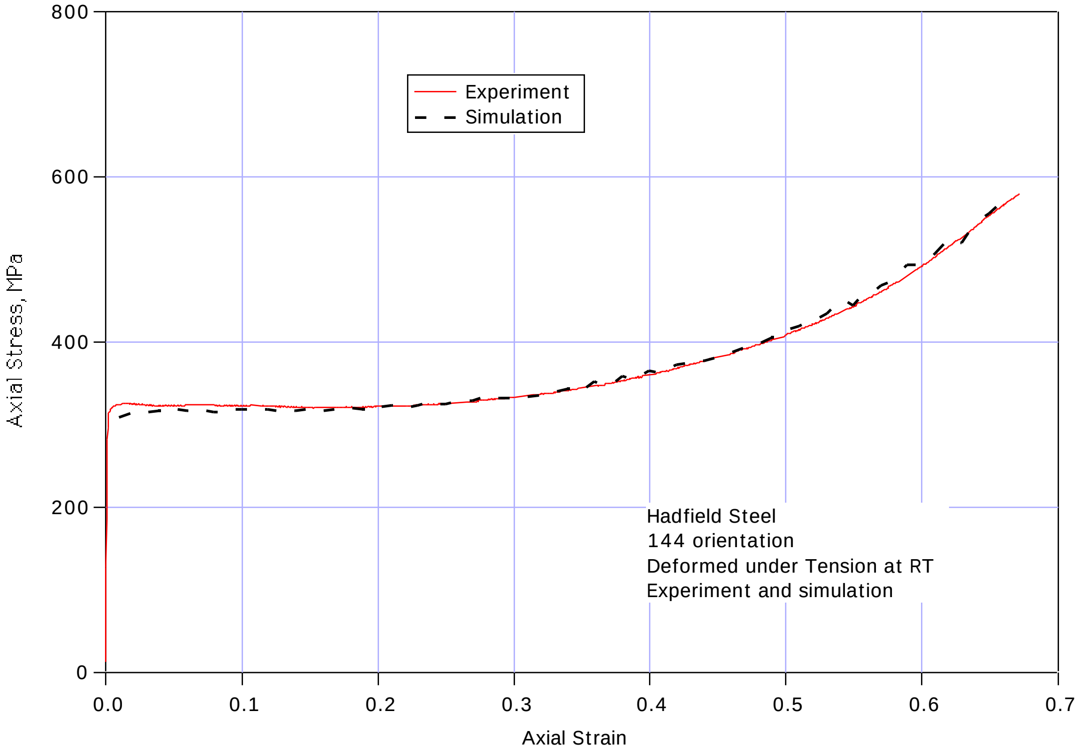
Modeling Results - [111] Orientation



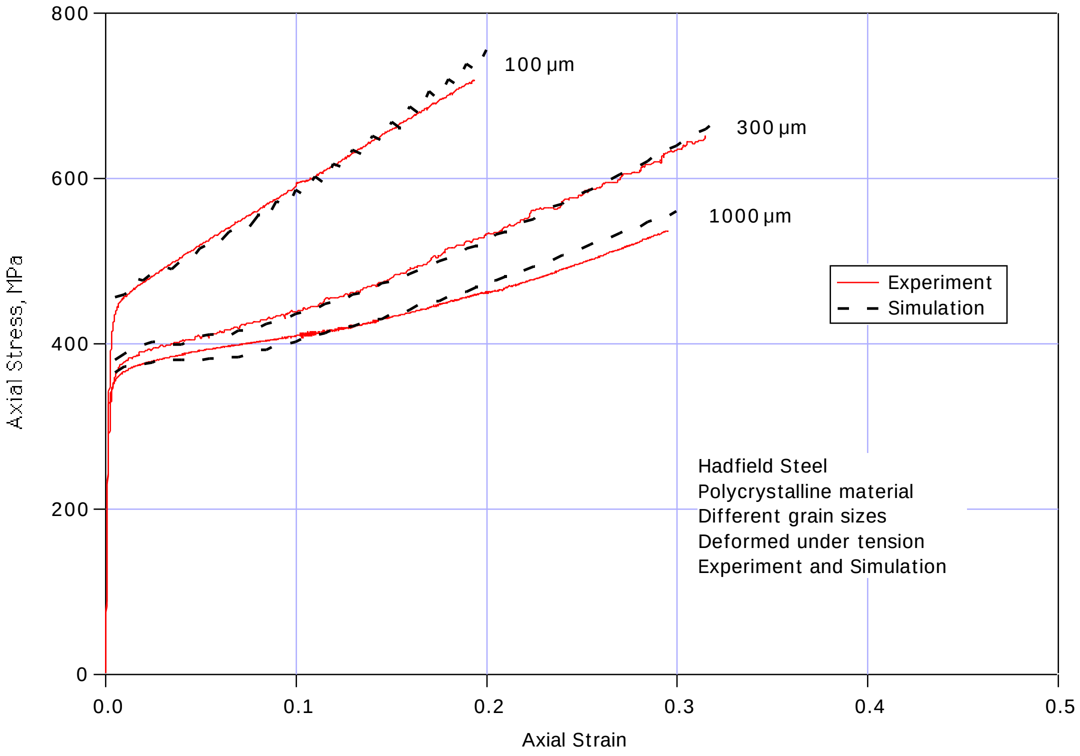
Hadfield Manganese Steel
[111] Orientation
Deformed under Tension at RT
Experiment and Simulation

Karaman, Sehitoglu, *et. al*, Acta Mat., 2000, Vol. 48, pp. 2031

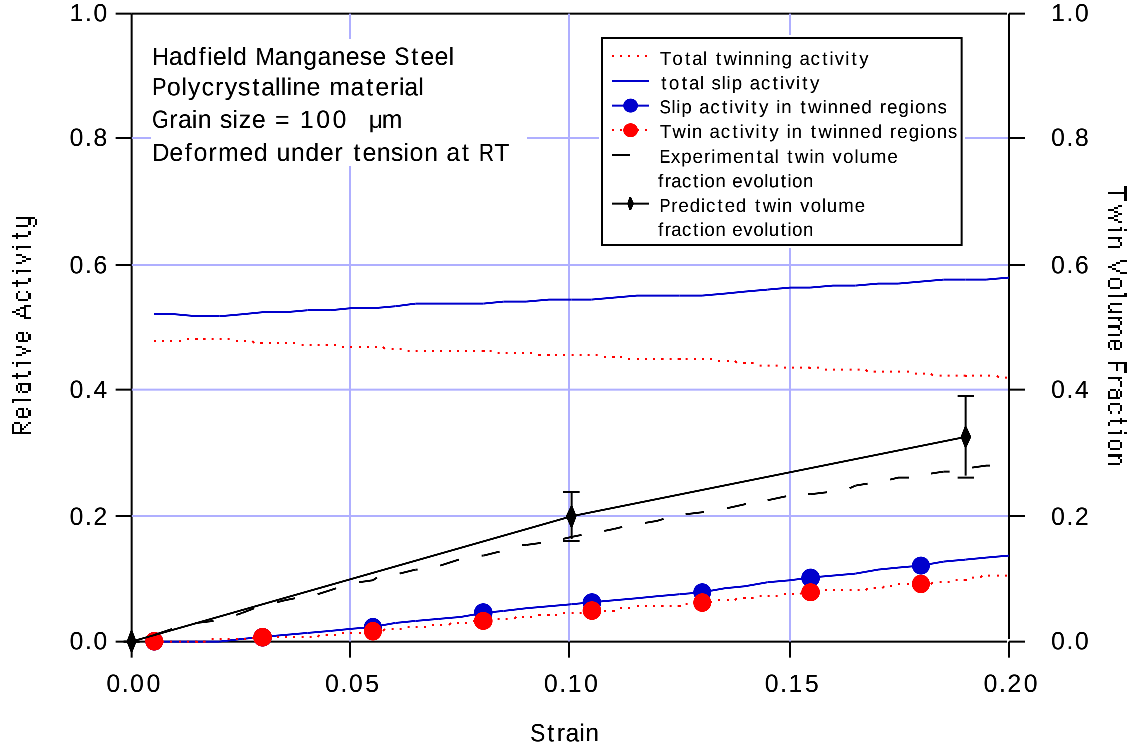
Modeling Results - [144] Orientation



Modeling Results - Effect of Grain Size



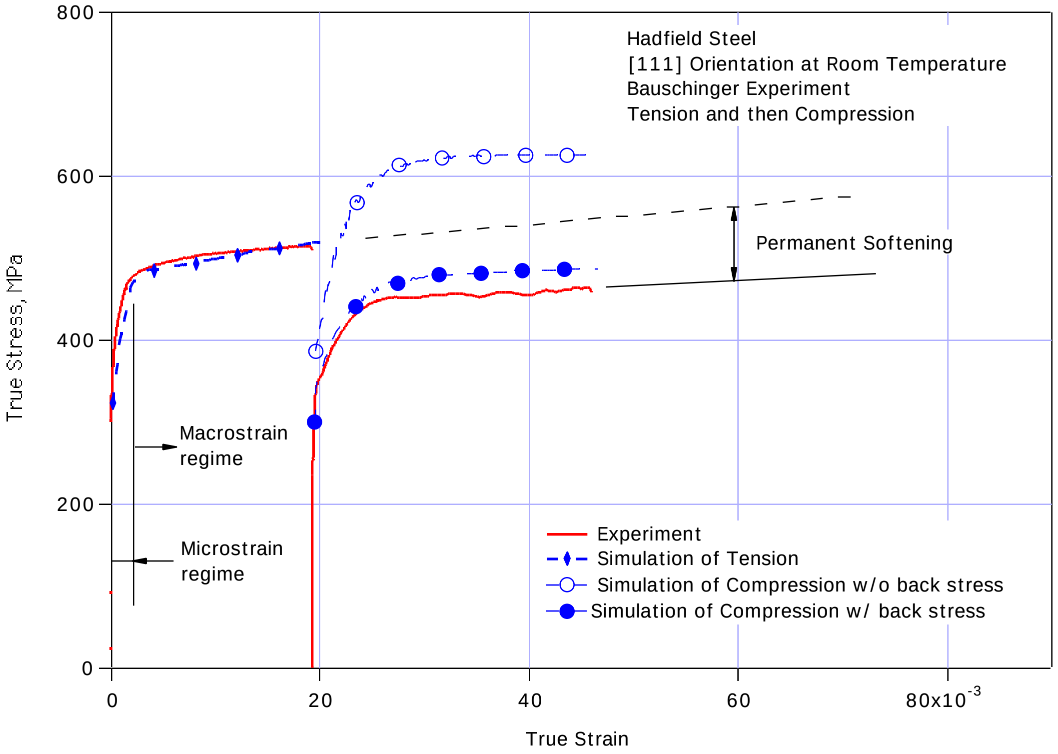
Modeling Results - Relative Activity and Volume Fraction Evolution



Summary of Modeling Efforts

- A new hardening law (physically sound with microscopic length scale, microstructure evolution and twin-slip interaction)
- Single crystal parameters -> Good prediction of polycrystalline materials.
- Twinning reorientation scheme predicts texture evolution

Bauschinger Experiments and Modeling



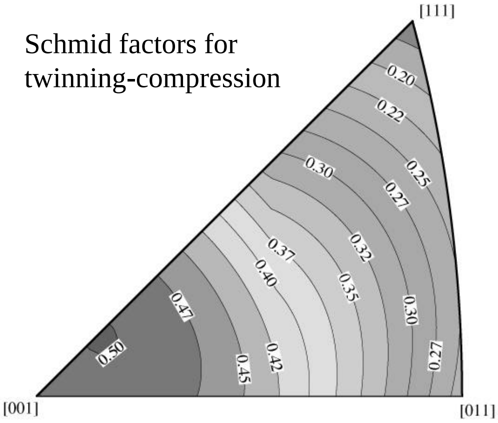
Karaman, I., H. Sehitoglu, Y. I. Chumlyakov, H. J. Maier, and I. V. Kireeva, *Metallurgical and Materials Transactions*, 32A:3 695_706, 2001.

Bauschinger Experiments (ctd.)

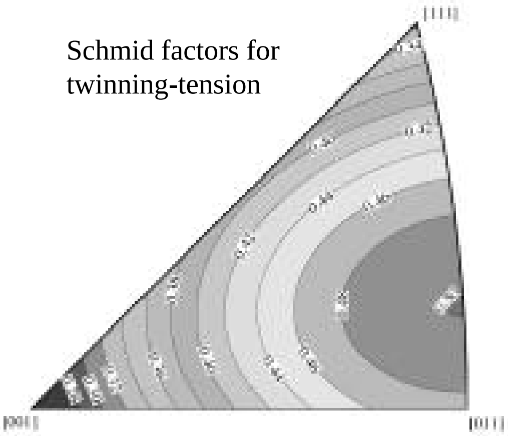
- Two different loading scheme

  FT/RC: Forward tension - reverse compression

  FC/RT: Forward compression - reverse tension

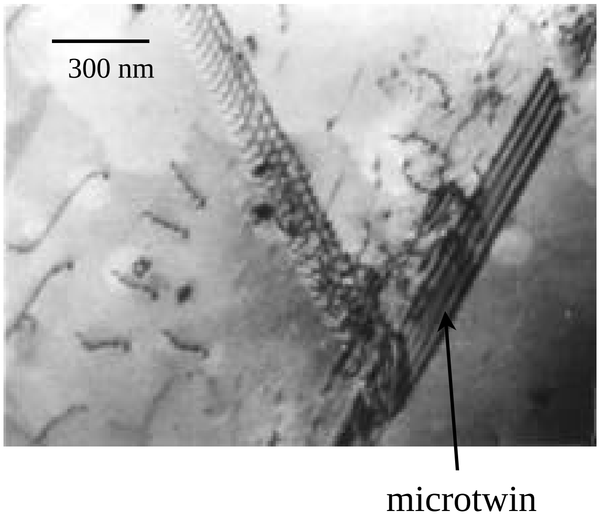


Schmid factors for twinning-compression



Schmid factors for twinning-tension

Twinning-Slip Interaction ([111] Orientation under tension)



Dislocation Pile-up leads to back stress that helps reverse yielding,

$$\sigma_f = \sigma_0 + \sigma_d + \sigma_b \quad \text{Forward Loading}$$

$$\sigma_f = \sigma_0 + \sigma_d - \sigma_b \quad \text{Reverse Loading}$$

Back stress can be calculated as

$$\sigma_{back} = 2\chi f \mu \varepsilon_p^* D$$

χ : Eshelby accomodation factor

f : Volume fraction of twins

ε_p^* : Unrelaxed shear strain

D : Modulus correction term due to twinning

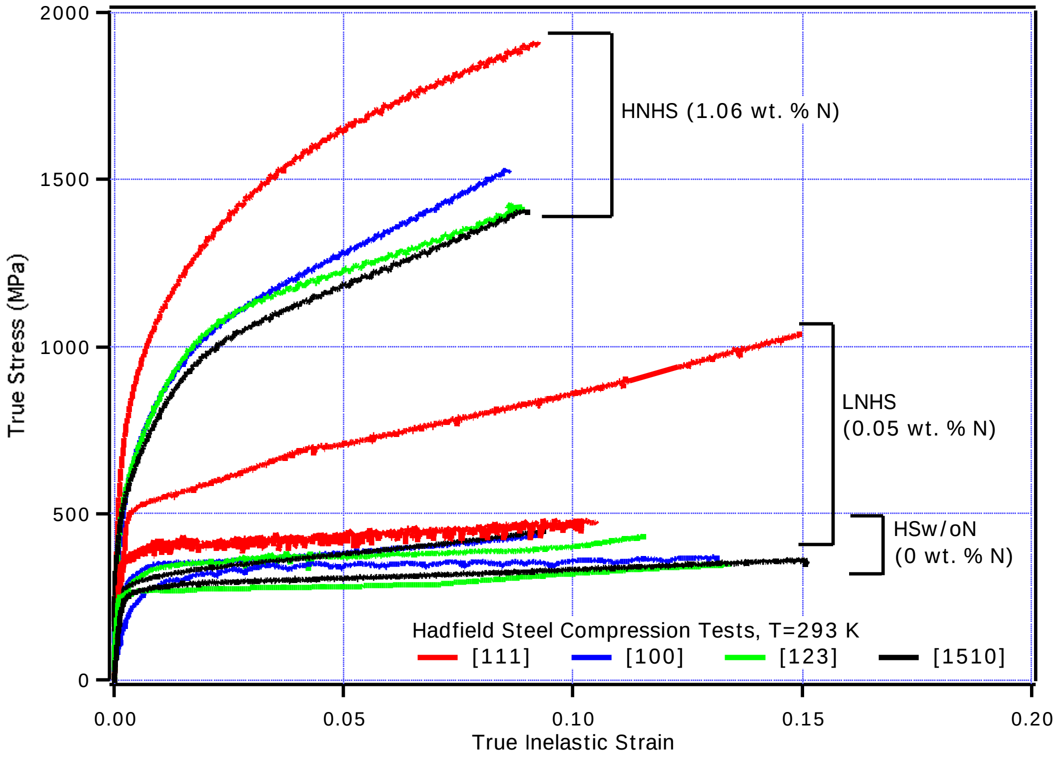
Summary- Bauschinger Effect

- High BE → long range internal stress originated by dislocation pileups accumulated at twinning and MSB boundaries. Twins and MSBs are hard but penetrable barriers.

- The Hadfield steel single crystals exhibit a higher BE that pure metal (Cu, Ni) and precipitation hardened Al-4Cu single crystals.

- The back stress and the strain hardening approaches correctly predicts the effect of volume fraction of twins and the number of active slip systems on BE in interstitial solid-solution hardened, low SFE steels.

Hadfield Steel with Nitrogen



Karaman, I., H. Sehitoglu, H. J. Maier, and Y. I. Chumlyakov,
Acta Materialia, 49:19 3919_3933, 2001.

Incorporation of Precipitation Hardening

- Precipitates are assumed to be elastic inclusions in the matrix.
- Average stress:

$$\hat{\tau} = (1 - f)\hat{\tau}^{m} + f\hat{\tau}^{p}$$

- Volume fraction of precipitates:

$$f^{p} = (2\pi / 3)(r / d_{3})^{2}$$

- The stress of the precipitate:

$$\hat{\tau}^{p} = 2\mu\chi D\gamma_{p}^{*}$$

- Plastic relaxation strain for spherical precipitates:

$$\gamma_{p}^{*} = \left(\frac{8\pi b}{\alpha^{2}\gamma_{p} r_{0}}\right)^{1/8} \alpha \left(\frac{8\gamma_{p} b}{\pi r_{0}}\right)^{1/2}$$

Constitutive Relation for Stress Evolution

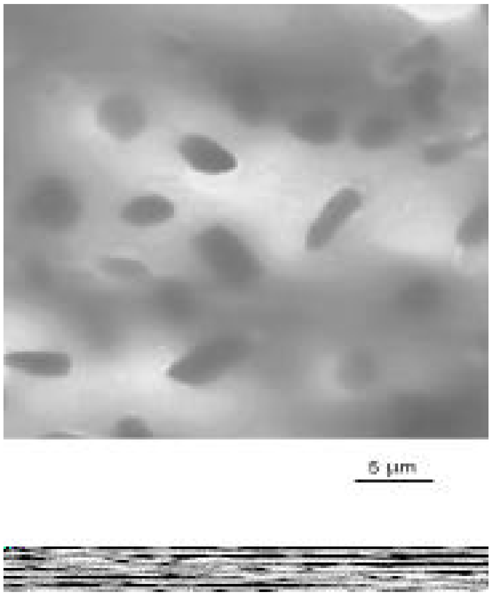
- Constitutive relation for stress evolution with plastic relaxation around particles:

$$\dot{\hat{\tau}} = \left[\left(1-\frac{2\pi}{3}\frac{r^2}{d_3^2}\right)\left(\frac{\alpha^2\mu^2 b}{2(\hat{\tau}-\hat{\tau}_0)}\sum_{s=1}^{2}\frac{K_s}{d_s}+\theta_0\left\{\frac{\hat{\tau}_s-\hat{\tau}}{\hat{\tau}_s-\tau_0}\right\}+\frac{\partial\hat{\tau}_i}{\partial\gamma}\right)+\pi\chi\frac{r^2}{d_3^2}\mu DA\frac{1}{\gamma^{5/8}}\right]\sum_k\left|\dot{\gamma}^k\right|$$

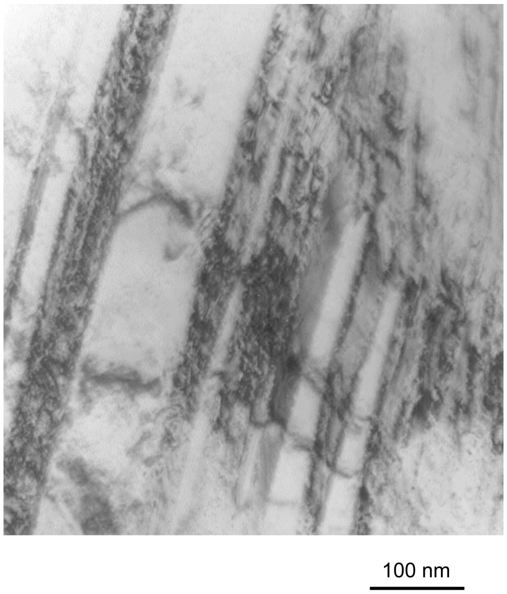
- Single crystal response:

$$\dot{\hat{\tau}} = \left[\left(1-\frac{2\pi}{3}\frac{r^2}{d_3^2}\right)\left(\frac{K_1\alpha^2\mu^2 b}{4(\hat{\tau}-\hat{\tau}_0)}\frac{1}{t}\frac{f^{tw}}{1-f^{tw}}+\frac{K_3\alpha^2\mu^2 b}{2(\hat{\tau}-\hat{\tau}_0)}\frac{1}{d_3}+\theta_0\left\{\frac{\hat{\tau}_s-\hat{\tau}}{\hat{\tau}_s-\tau_0}\right\}+\frac{\partial\hat{\tau}_i}{\partial\gamma}\right)+\pi\chi\frac{r_0^2}{d_3^2}\mu DA\frac{1}{\gamma^{5/8}}\right]\sum_k\left|\dot{\gamma}^k\right|$$

Microstructure - HNHS

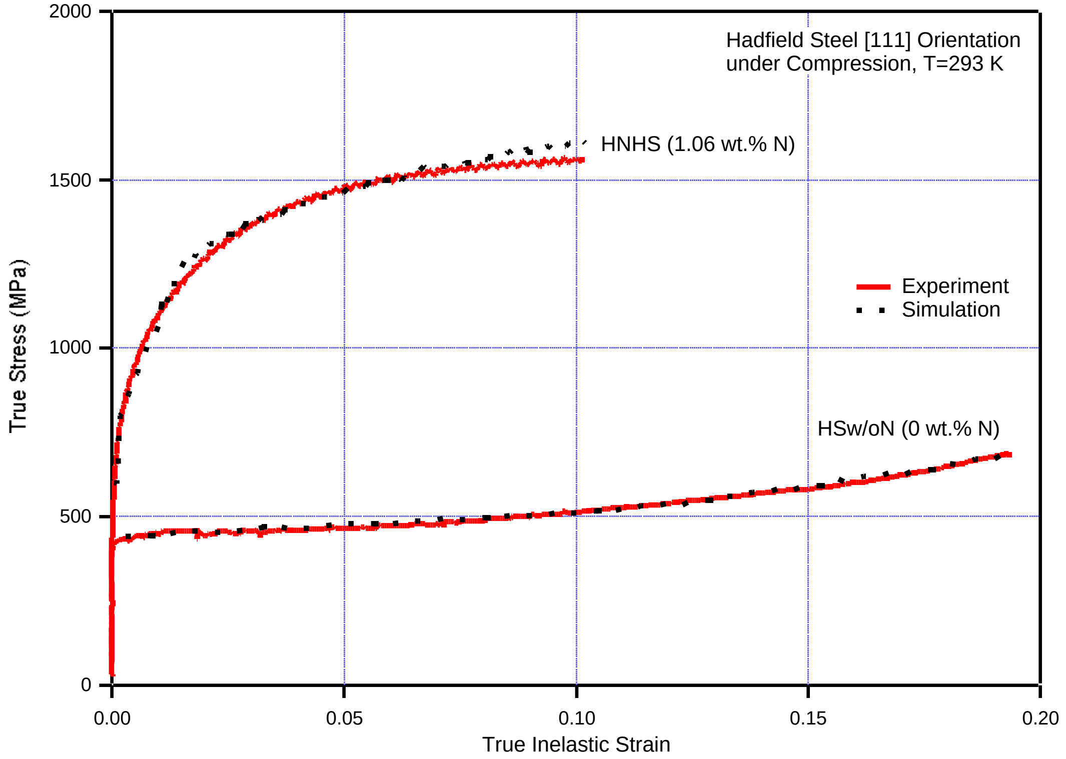


HNHS [111] at 5% strain.

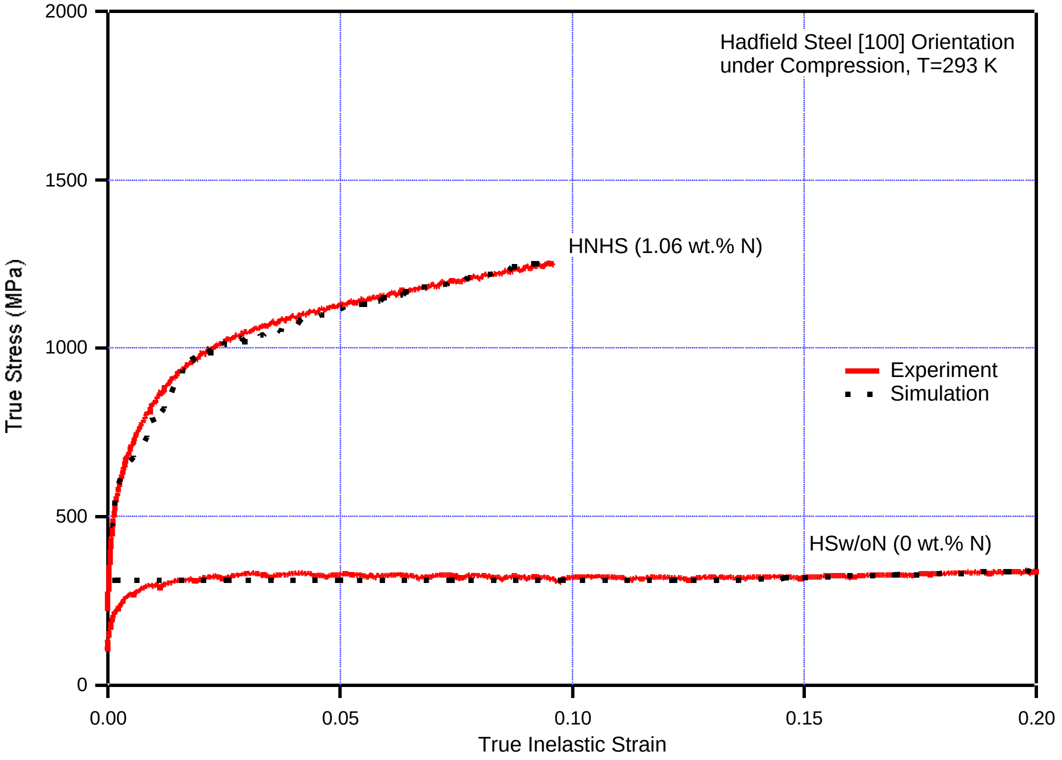


HNHS [1510] at 22% strain.

Theory vs. Experiment - [111] Orientation



Theory vs. Experiment - [100] Orientation



Summary- High Nitrogen Effects

The addition of nitrogen resulted in a drastic increase in yield strength levels. Increasing twin density in the microstructure results in an increase in the deformation hardening in the presence of precipitates.

A visco-plastic self-consistent (VPSC) model was modified to account for precipitation and twinning length scales in Hadfield steel with and without nitrogen. The model showed that it is feasible to treat both coherent and incoherent precipitates in the hardening formulation as factors affecting the mean free path of dislocations.