Multiscale Models and Methods: Hierarchical Multi-scale Modeling of Irradiation Induced Strengthening

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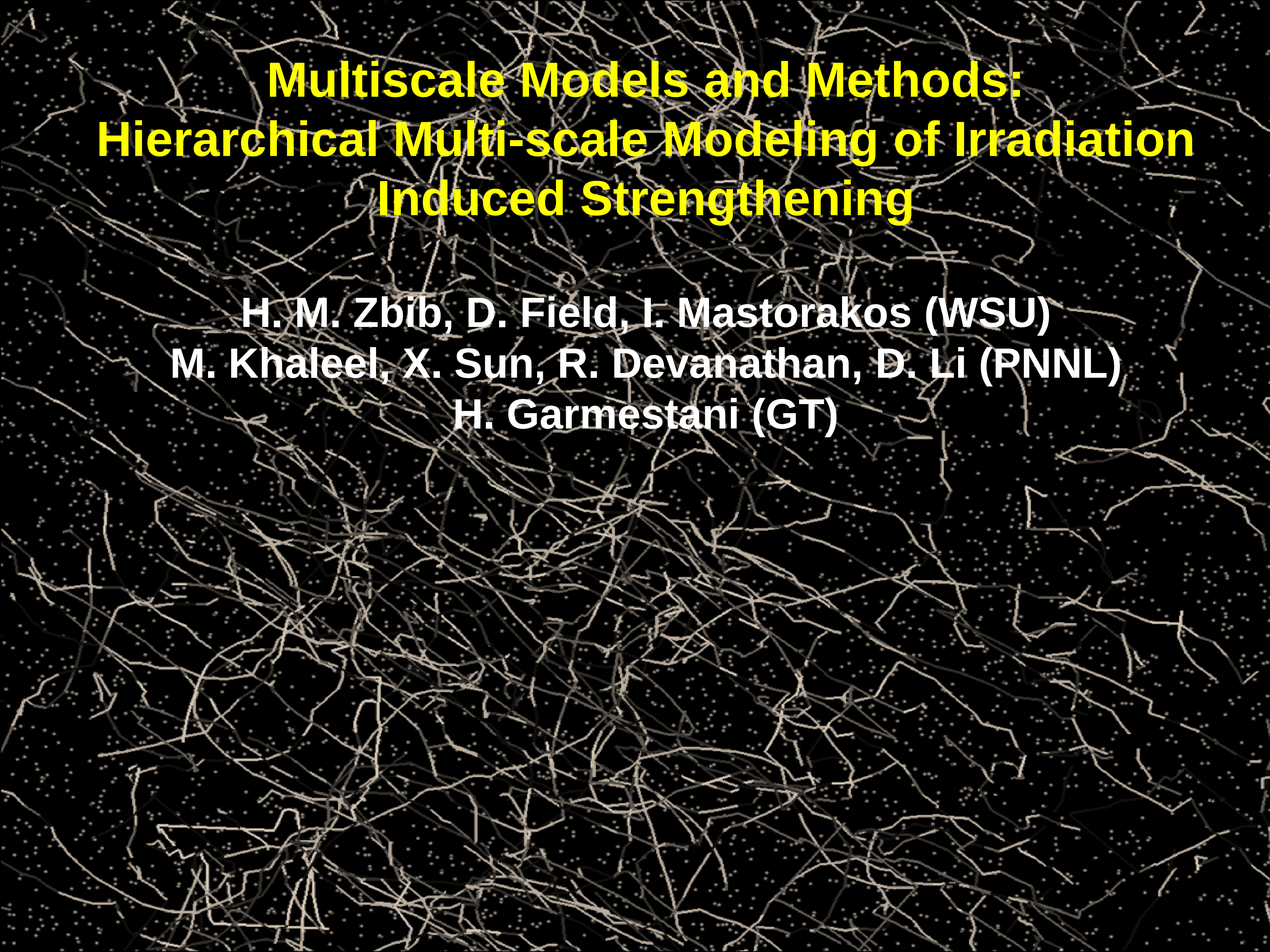
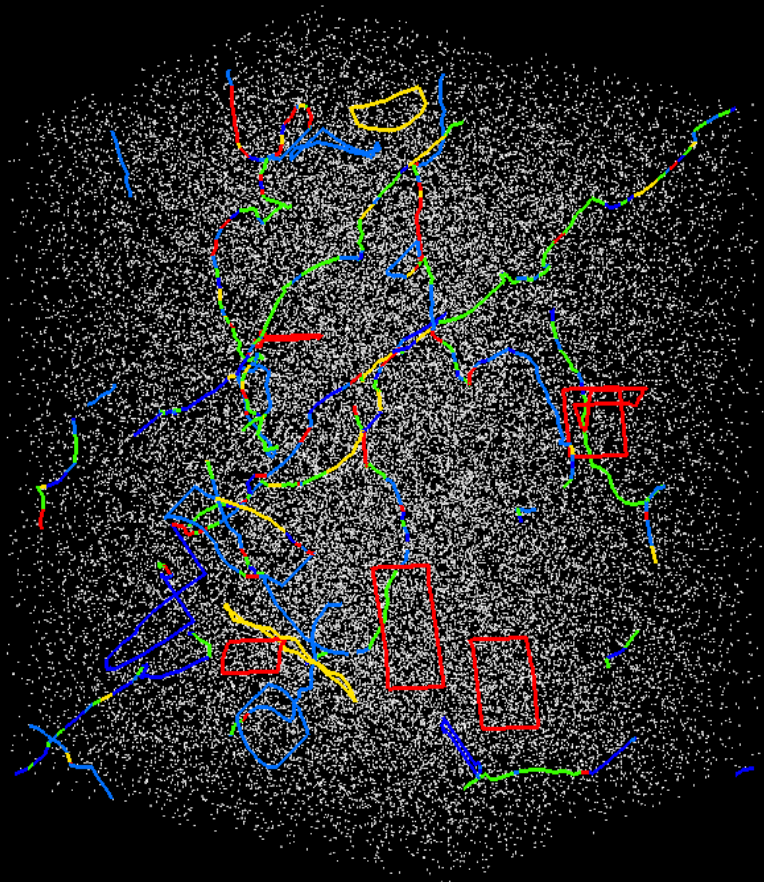


Objective:

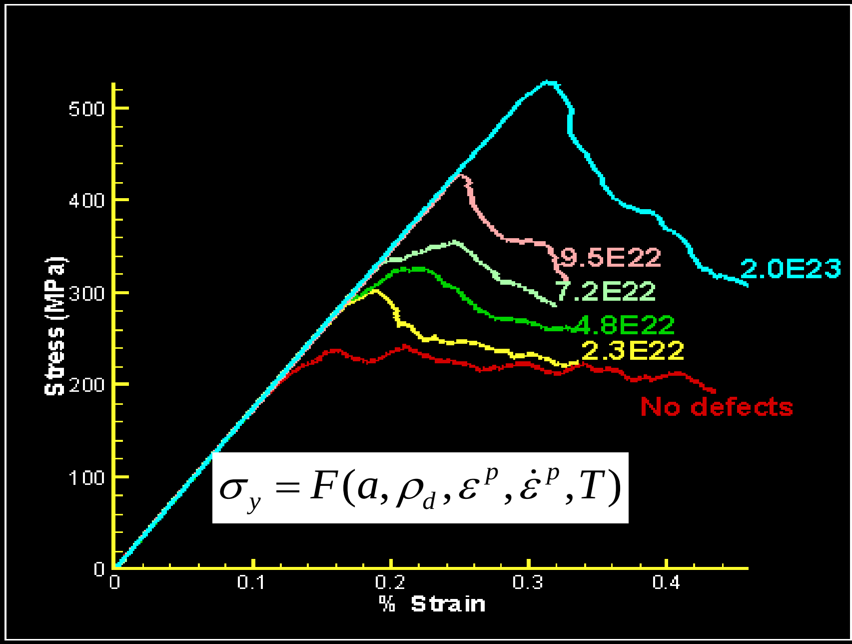
To develop a physically-based capability that predicts aging behavior and performance and in-service lifetime of structural materials used in nuclear reactors with focus on advanced steels.

Outcomes:

Physically-based strength models, evolution laws and data base for use in the integrated codes.



Developed **numerical methods**
to pass information between length scales:
nano to micro to meso
MD-DD-CP



Developing data base and Strength **models** as a function of composition, microstructure, environment

Ferritic-Martensitic steels

have excellent 100,000 hour creep lives, are widely used in the thermal power generation industry where operational temperatures are in the neighborhood of 550ºC and above. Compositional modifications of conventional 9-12% Cr steels (e.g. Mo, W, V, N) have been introduced (such as in T91/92 and P91/92) which allow for increases in operating temperatures that exceed 600ºC.

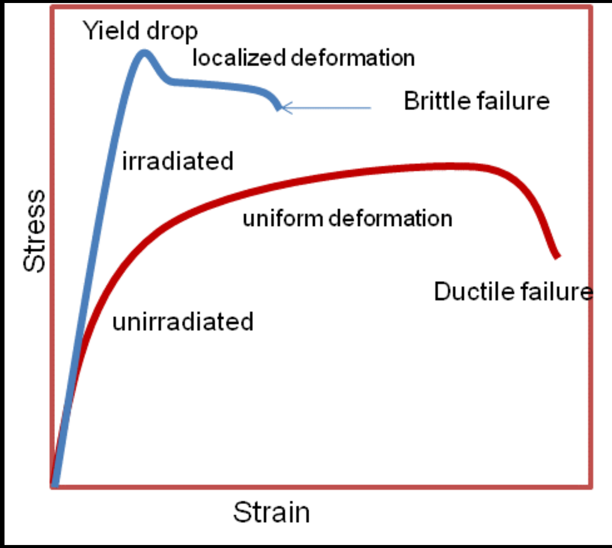
Ferritic-Martensitic steels

✓Have good resistant to swelling & maintain good fracture toughness at irradiation above 673K.

✓At low to intermediate temperatures (T < ≈550 °C), they are prone to loss of ductility, increase yield stress, reduce strain hardening capacity & flow localization.

✓The predominant microstructural features are very small (≈ nm) cluster-type features:
Dislocation loops, Cavities, Regions of solute segregation and 2nd phase precipitates.

✓The balance of these features depends on the synergistic interaction of key irradiation, material and environmental variables, such as irradiation temperature, dose and dose rate, defect, and **alloy composition**.



Degradation of properties is driven by changes in microstructure that are driven by radiation environment, temperature, pressure, etc.

Materials Challenge:

Develop accurate life prediction models that account for:

> High Irradiation
> High/cyclic temperature (start-up and shut down events)
> Variations in steady state operating conditions

Also

> Hostile media (oxygen, water, hydrogen (radiolysis), galvanic corrosion)
> Hydrostatic pressure
> Others…

Current designs are based n extrapolation of data from short-term tests to predict the lifetime and reliability of structural components.

Predictive modeling can improve upon this.

Fundamentals:

The effect of environment on materials microstructure and mechanical properties is an inherently multiscale phenomenon involving processes spanning a wide range of length and time scales.

We have been working on three major interrelated tasks.

Molecular Dynamics simulations*, over a wide range of parameter space, of point defects and defect clusters, helium, hydrogen formation and annihilation; defect-grain boundary interaction, dislocation-defect-grain boundary interaction, and dislocation solute interaction and dislocation mobility as a function of solute atom concentration.*

Dislocation dynamics simulations, over a wide range of parameter space of defect cluster density, helium density, and dislocation density. This also includes the development of models for climb processes based in input from MD.

Crystal plasticity (CP) modeling and simulations*. This includes the development of models for grain boundaries and hardening laws that account for irradiation effect based on input form DD and MD.*

Summary of accomplishments so far..

- Developed data (MD-based) for

  Dislocation mobility and

  Dislocation/defect/precipitate interaction

  for different compositions of Fe-%Cr and Fe-%Ni.

- Developed a methodology for determining hardening laws, coupling MD-DD-CP

- Developing code for obtaining minimum energy grain boundary structures. Building a database of Fe grain boundary structures

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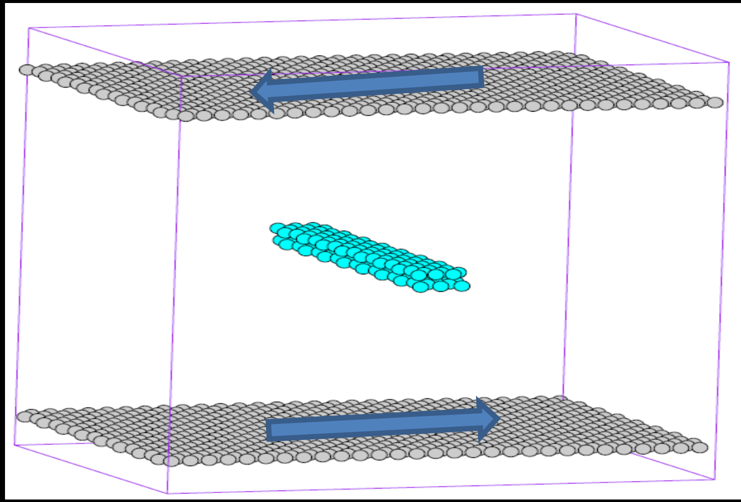
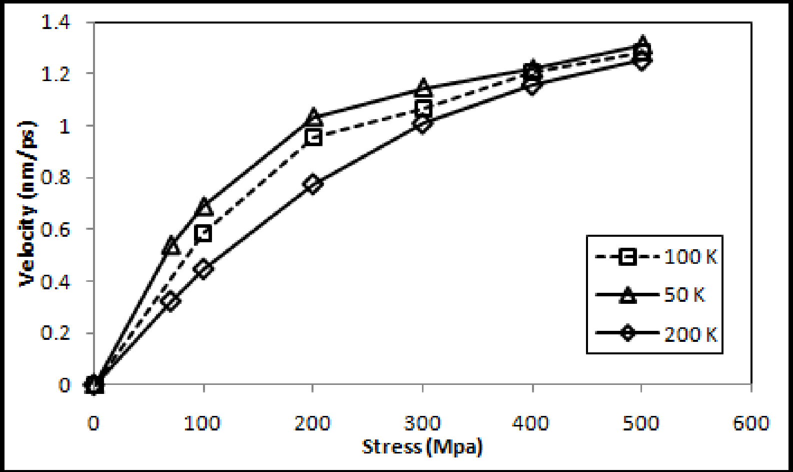
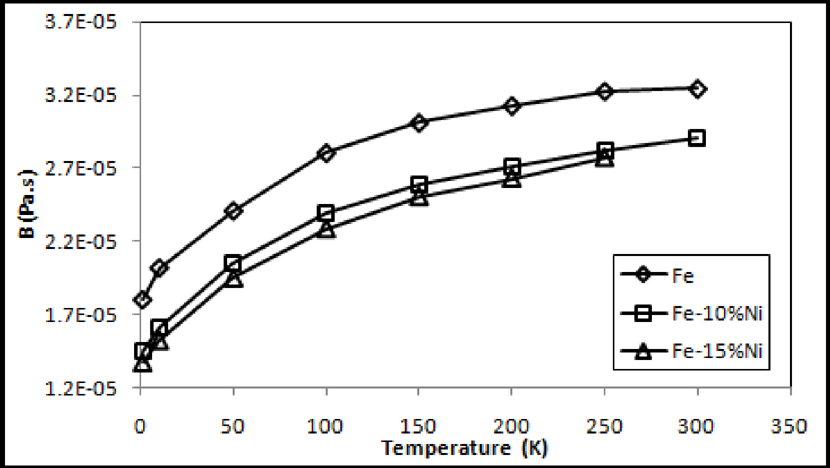
Dislocation mobility





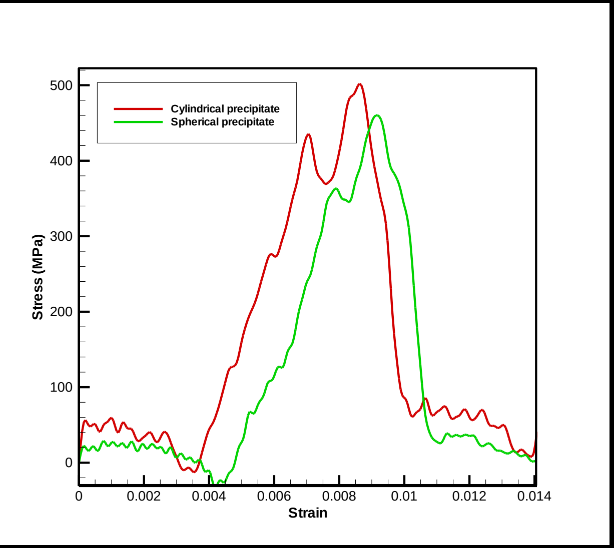
Dislocation velocity vs. applied stress for a-Fe (various temperatures)

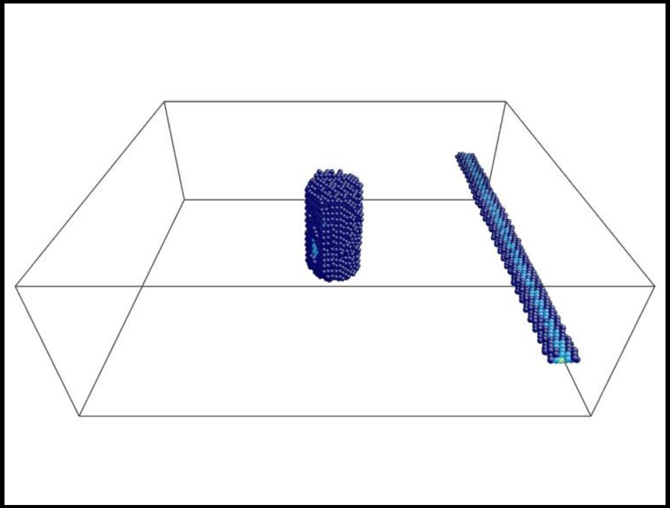


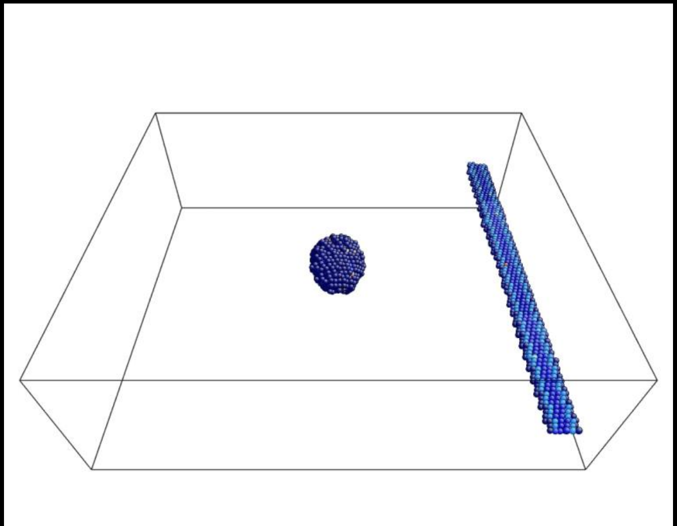
Dislocation damping constant vs. temperature (various Ni concentrations)

MD: Dislocation – Ni Precipitate interaction in Fe

Precipitate – dislocation collision:
The precipitate acts as an obstacle to the dislocation motion. The mechanism is independent on the shape of the precipitate, but not the critical stress.

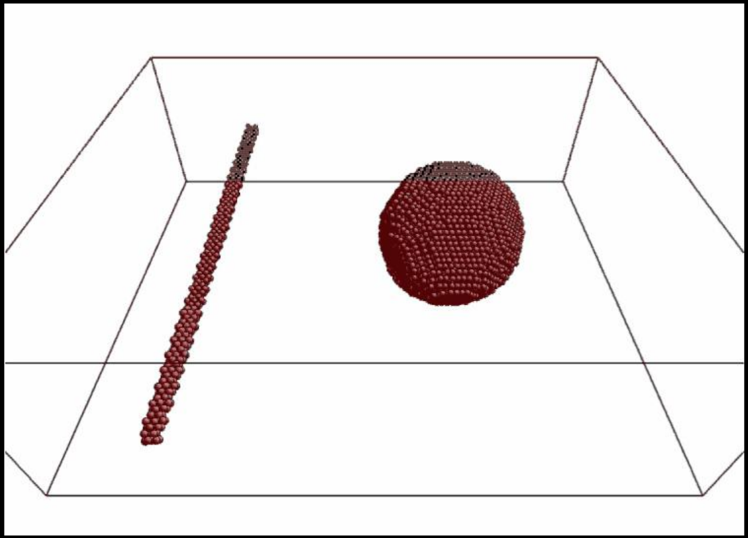


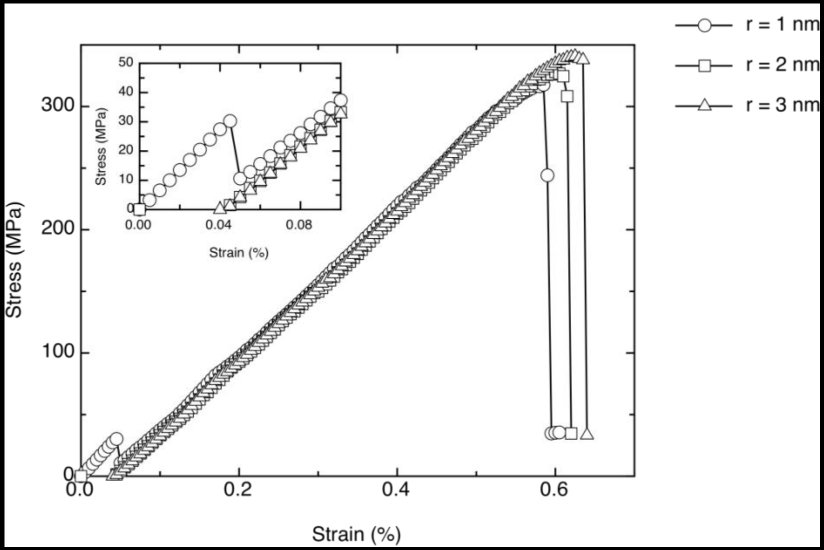




Dislocation – Void collision in a-Fe

Void – dislocation collision: The effect of void size. The void acts as an obstacle to dislocation motion. The stress increases in a logarithmic fashion as the void size increases





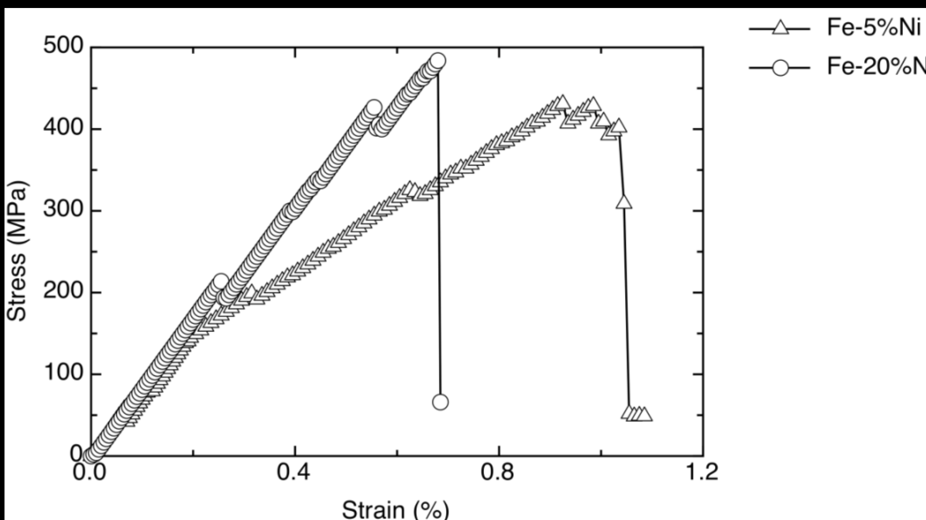
$$\sigma = \sigma_0 + \frac{\alpha\mu}{2\pi}\frac{1}{W^n}\ln\left(\frac{\beta D}{b}\right)$$

CRSS as a function of void diameter D, and spacing W

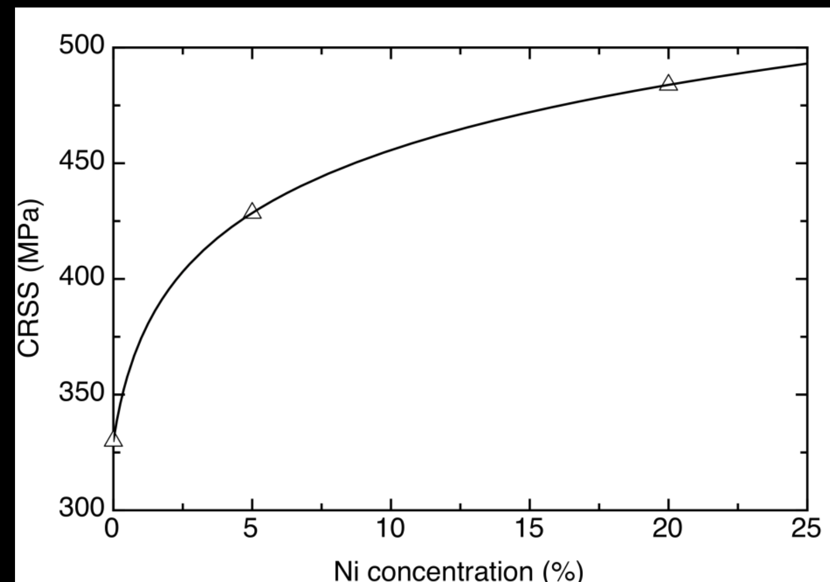
Fitting parameters: α = 4.08, β = 1.3 and n = 1.12

Dislocation – Void collision in Fe-Ni (work in progress)

Void – dislocation collision: The effect of Ni concentration on the CRSS
The addition of Ni increases the CRSS for a given void size



Stress – strain curves for the case 4 nm void diameter



CRSS as a function of % Ni concentration

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Data base

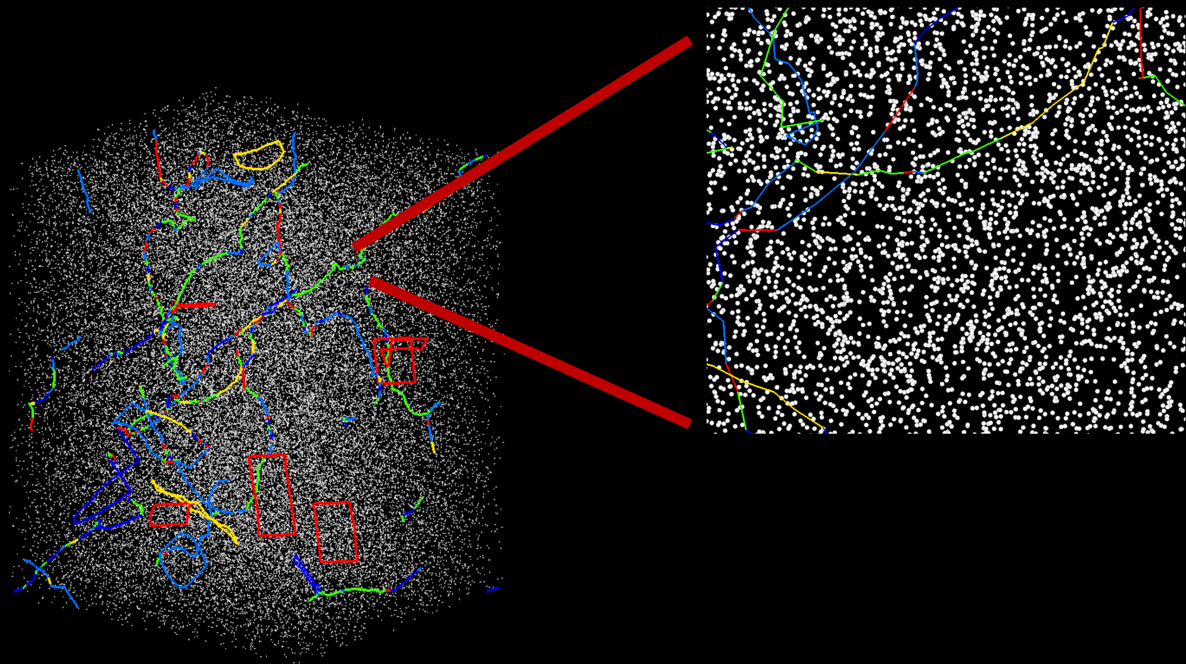
Dislocation dynamics simulations, over a wide range of parameter space of defect cluster density, helium density, and dislocation density. This also includes the development of models for climb processes based in input from MD.

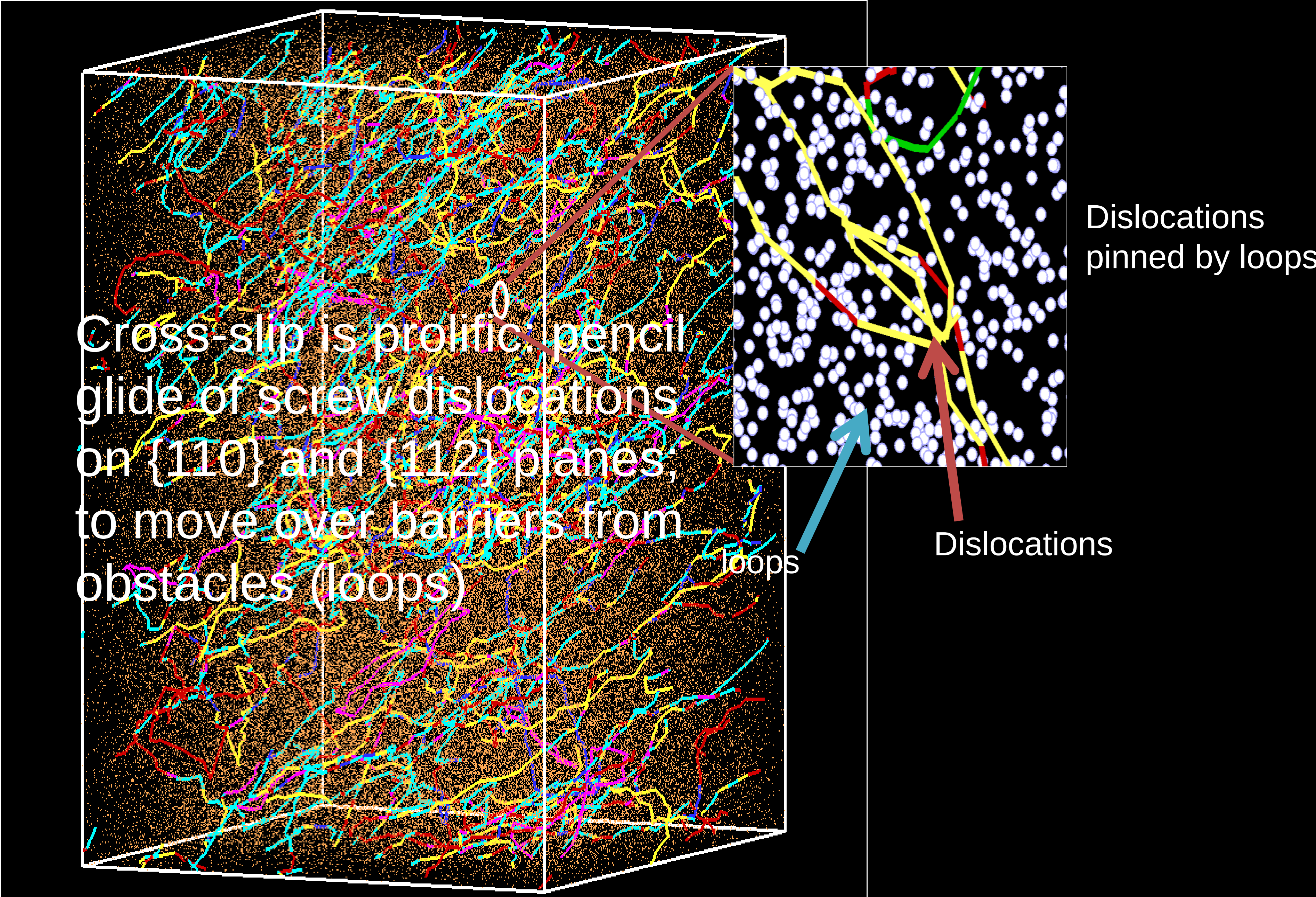
Crystal plasticity (CP) modeling and simulations. This includes the development of models for grain boundaries and hardening laws that account for irradiation effect based on input form DD and MD.

Dislocation dynamics (DD) -microscale:

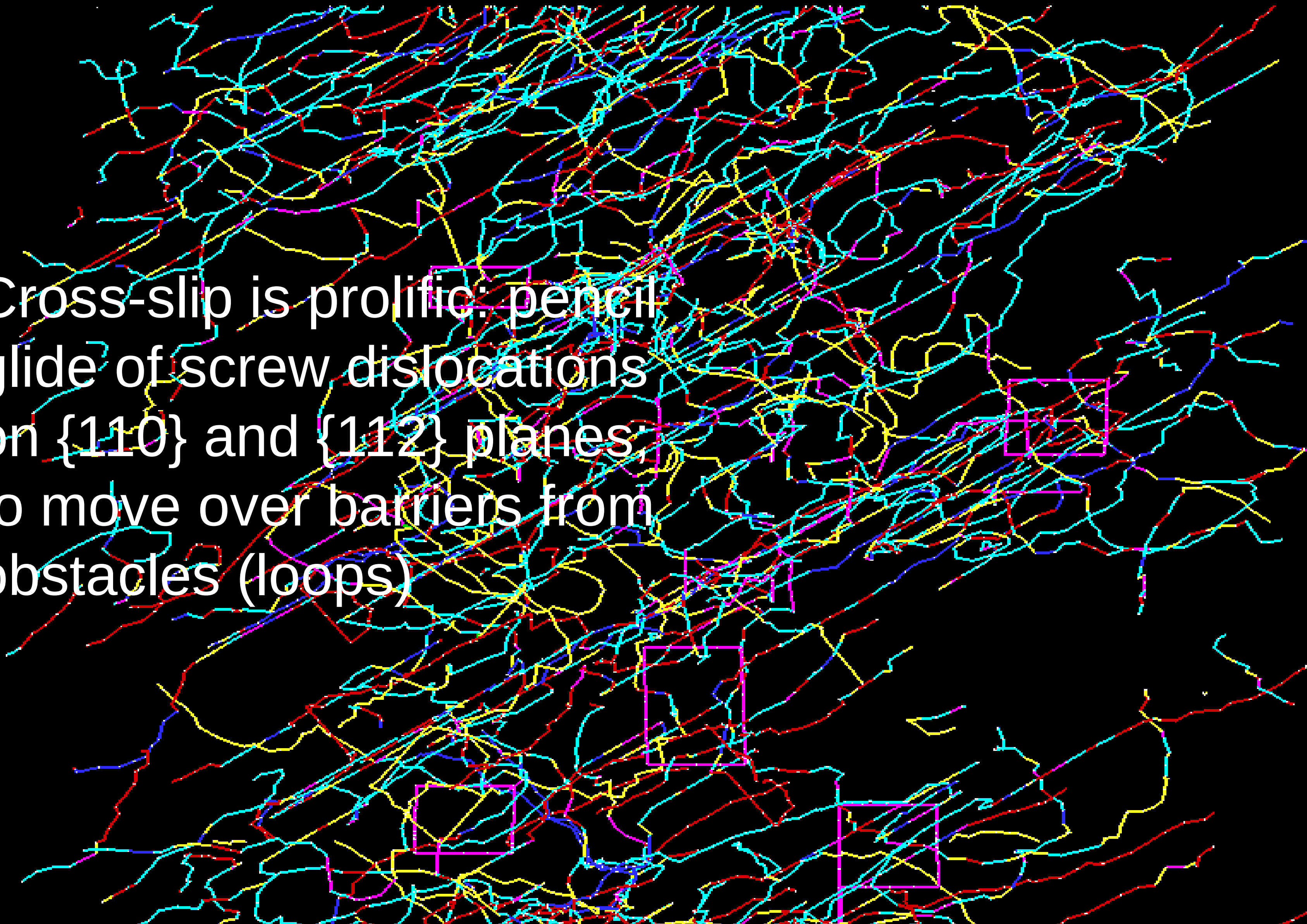
Collective behavior of an ensemble of dislocations & defects; predict deformation, strength, and defect evolution

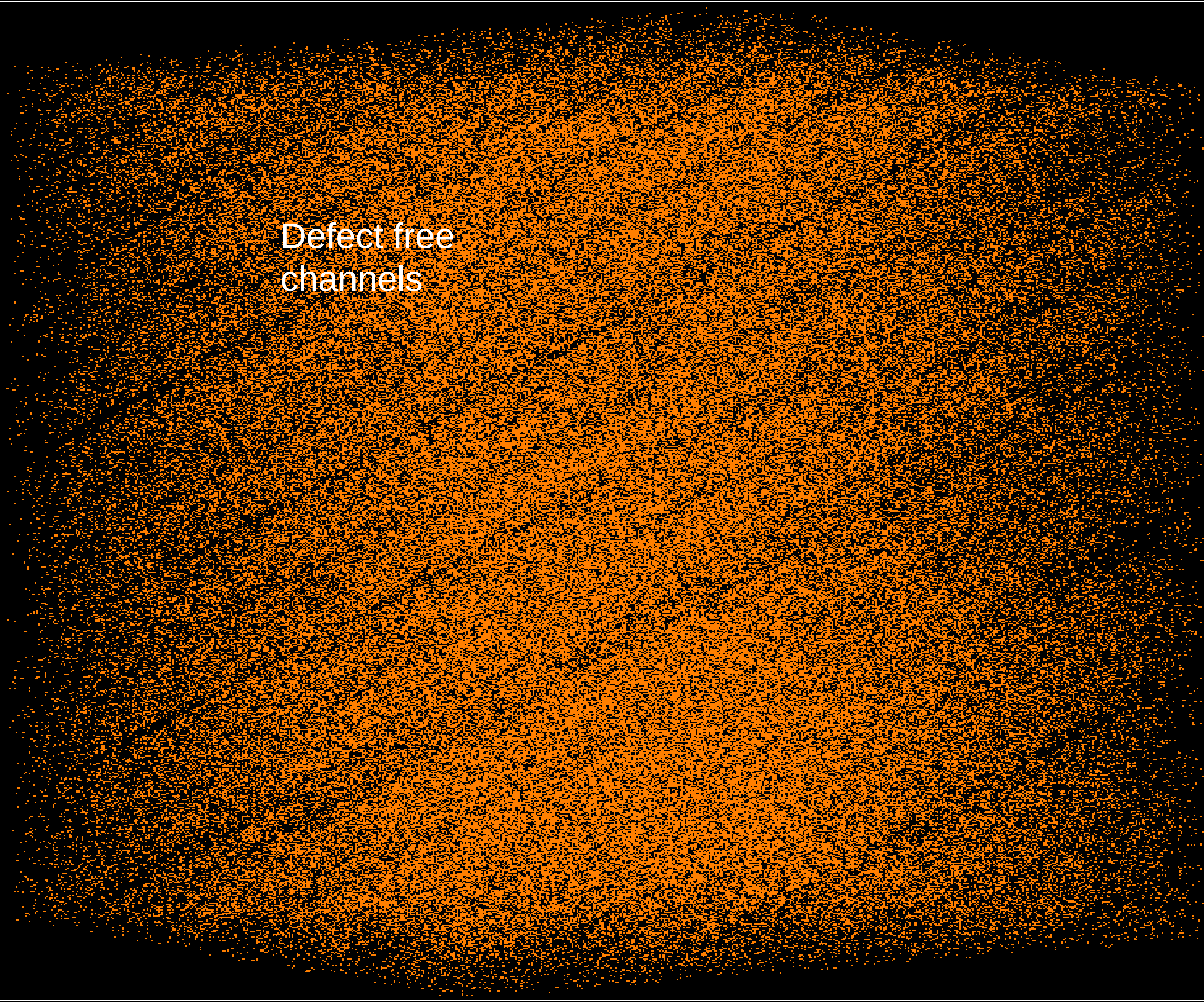
Fe -%Cr/Ni
Tension,
3.38μmX3.38μmx4.47μm sample
Random distribution of Dislocation sources
Defect density: $8X10^{20}$ to $2x10^{23}$ /m^3
<100> and <111> FS loops
Periodic boundary conditions
Coupled DD-FE

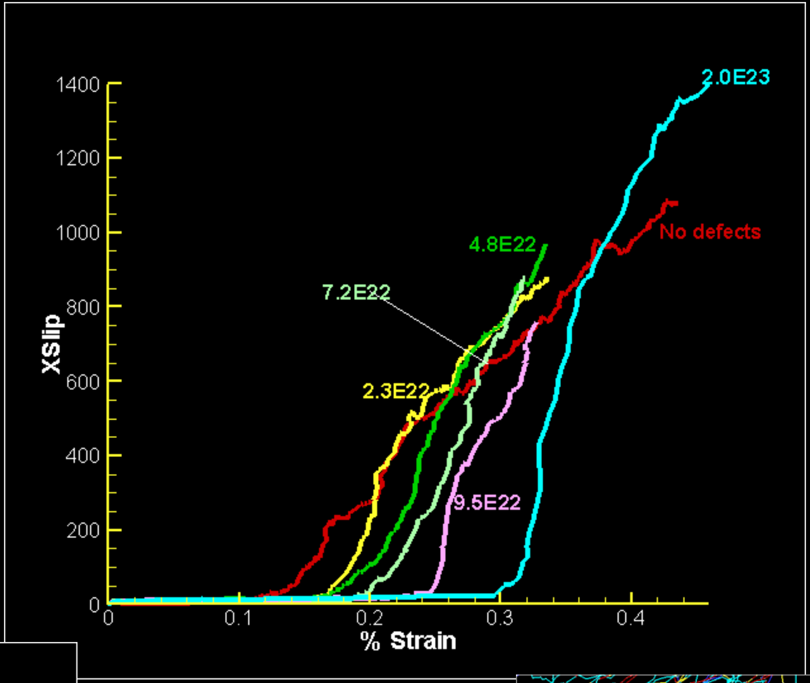


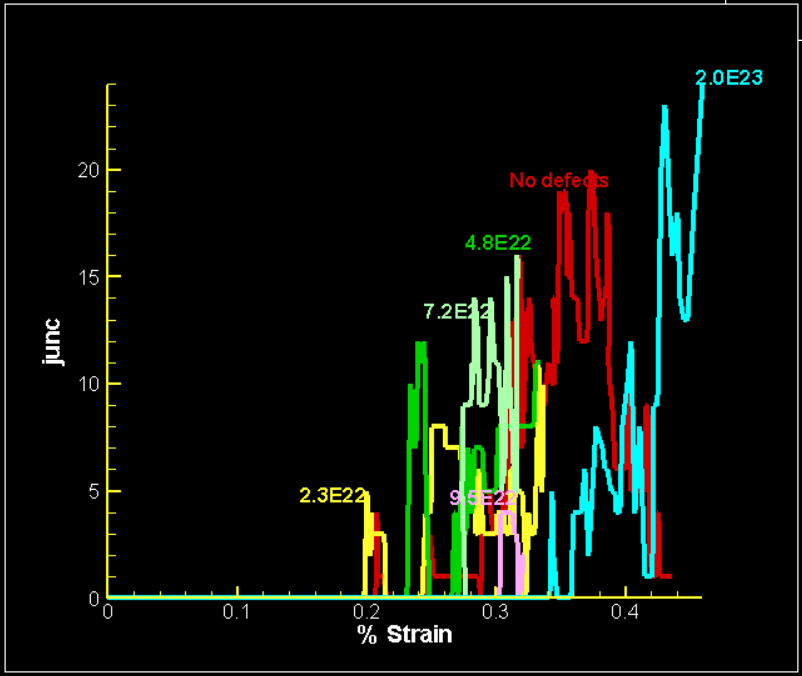

Cross-slip is prolific: pencil glide of screw dislocations on {110} and {112} planes; to move over barriers from obstacles (loops)
Dislocations pinned by loops
loops
Dislocations

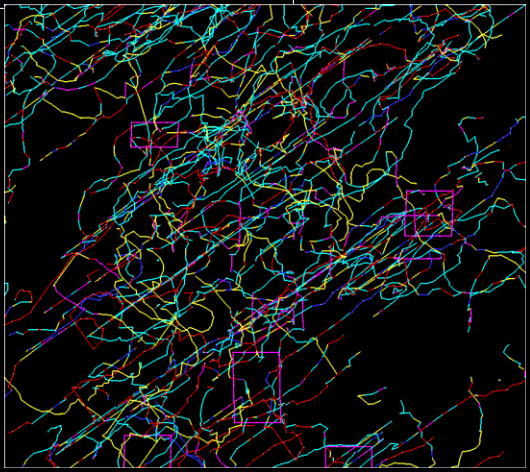
Cross-slip is prolific: pencil glide of screw dislocations on {110} and {112} planes; to move over barriers from obstacles (loops)

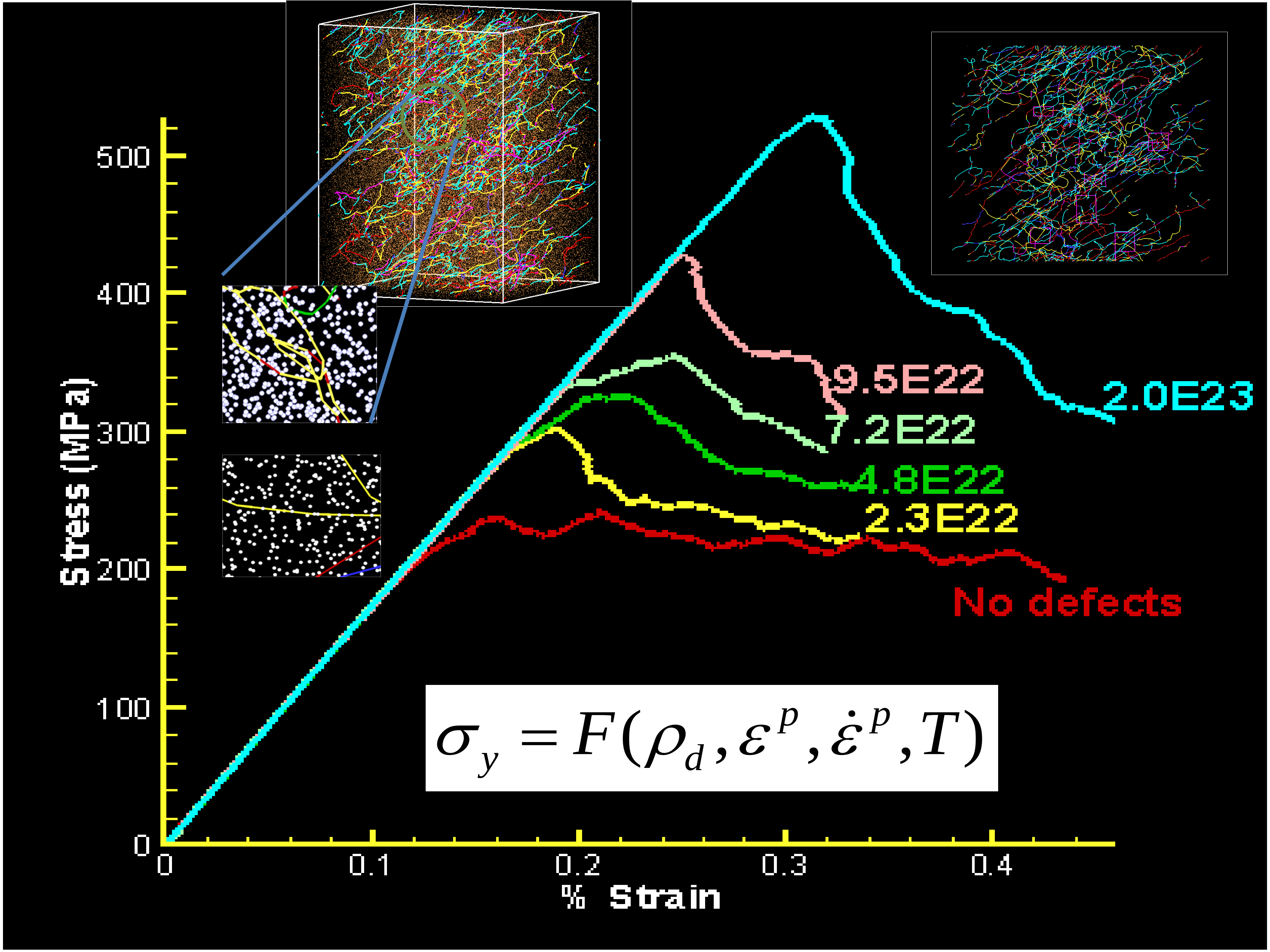



Defect free
channels

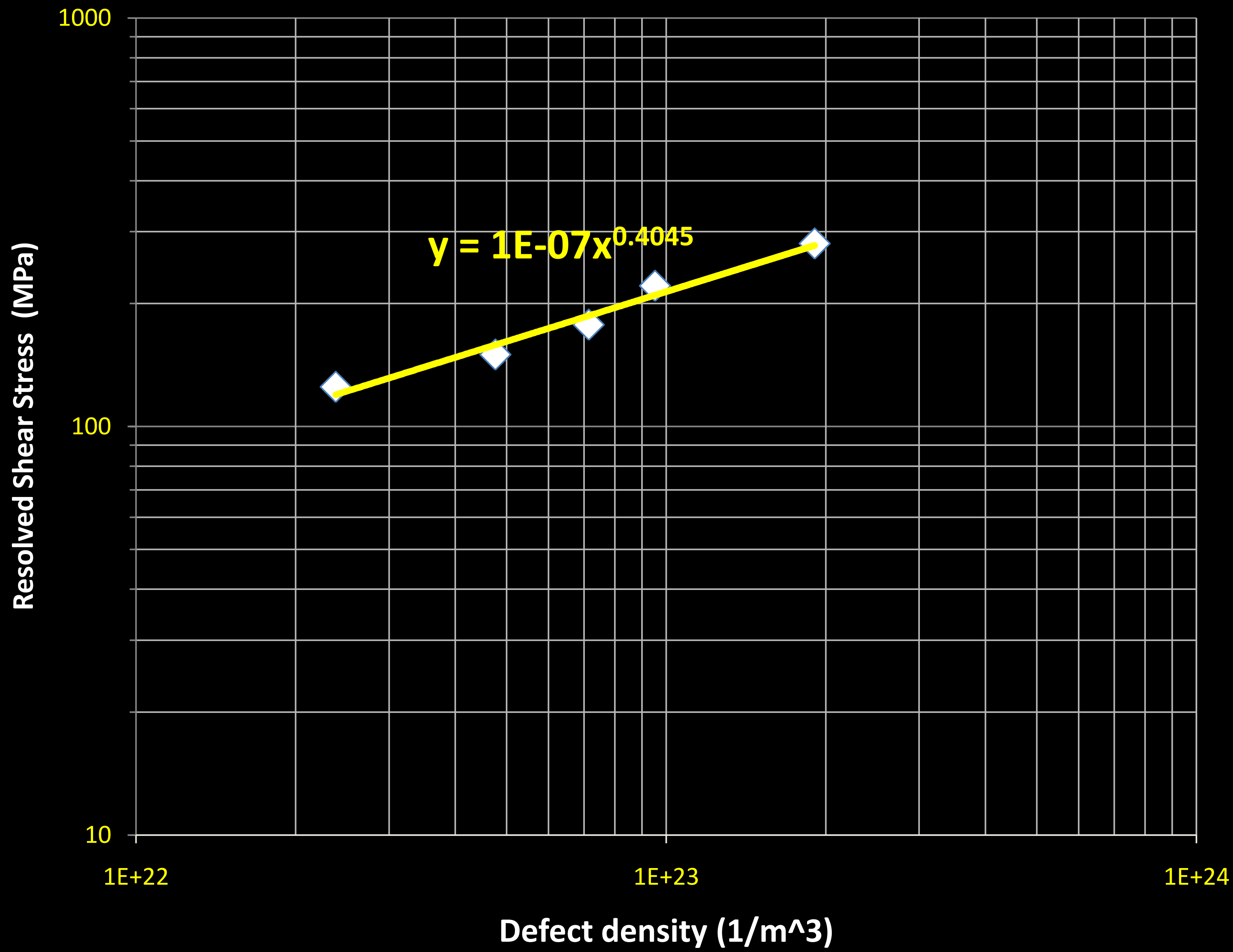

2.0E23
No defects
4.8E22
7.2E22
2.3E22
9.5E22
XSlip
1400
1200
1000
800
600
400
200
0
0
0.1
0.2
0.3
0.4
% Strain


2.0E23
No defects
4.8E22
7.2E22
2.3E22
9.5E22
junc
20
15
10
5
0
0
0.1
0.2
0.3
0.4
% Strain



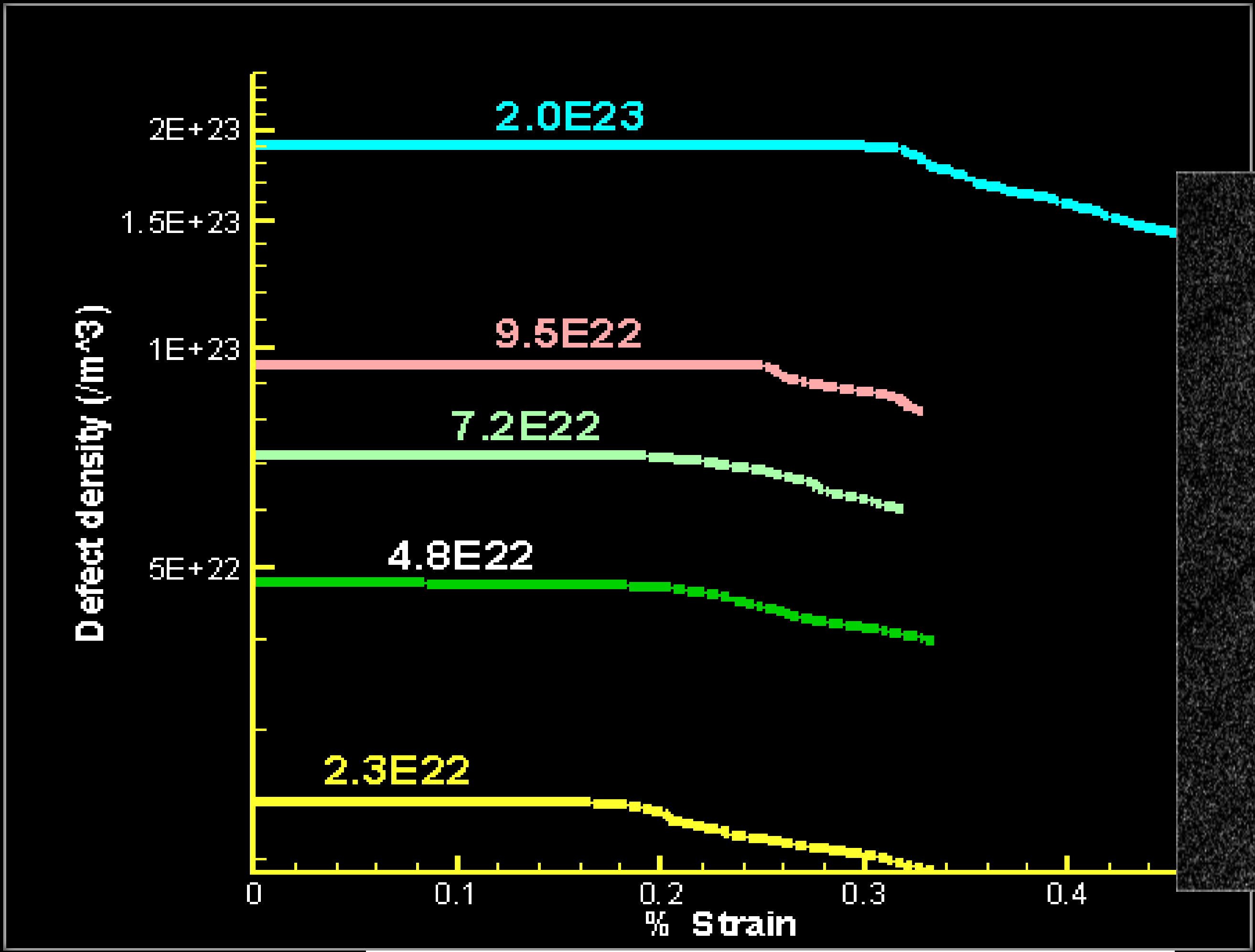


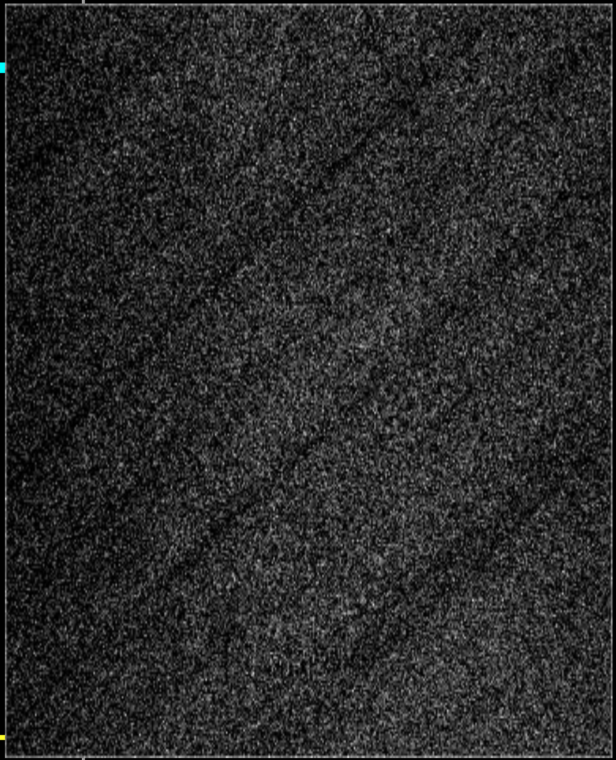
$$\sigma_y = F(\rho_d, \varepsilon^p, \dot{\varepsilon}^p, T)$$



y = 1E-07x^0.4045
1000
100
10
Resolved Shear Stress (MPa)
1E+22
1E+23
1E+24
Defect density (1/m^3)

Clearing of defects; leads to strain-softening and localized deformation



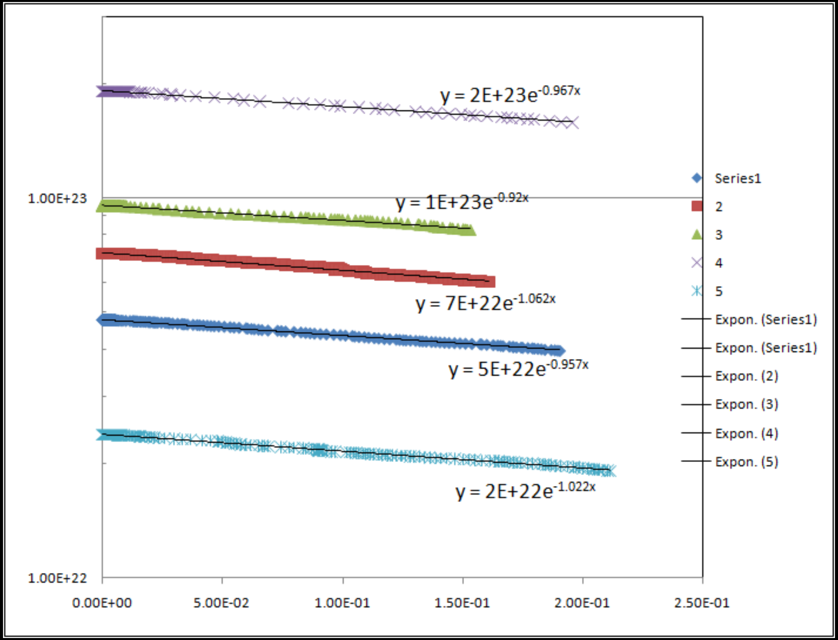


$$\dot{\rho}_d = G(\dot{\varepsilon}^p, \rho_d, R_c, T)$$

$\rho_d = \#\,defects\,/\,volume$

Model:
n = Total number of defects in a region of radius R (capture radius for dislocation-loop interaction)
t = time for one dislocation to move through region R
f= frequency of N defects interacting with one dislocation sweeping through R

$$\dot{\rho}_d = -\beta\pi\frac{R}{b}\rho_d\dot{\gamma}$$



Strong dependence on defect type, distributions, capture radius, and frequency of encounter between dislocations

Statistical Spatial correlation distribution functions are determined from Dislocation Dynamics Simulations

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Dislocation dynamics simulations, over a wide range of parameter space of defect cluster density, helium density, and dislocation density. This also includes the development of models for climb processes based in input from MD.

Results to pass to meso-macro models?

Depends on the model.

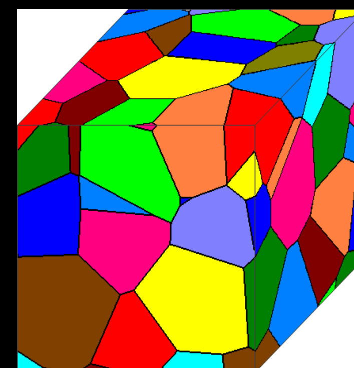
Hardening laws: Local versus nonlocal

Crystal plasticity (CP) modeling and simulations. This includes the development of models for grain boundaries and hardening laws that account for irradiation effect based on input form DD and MD.

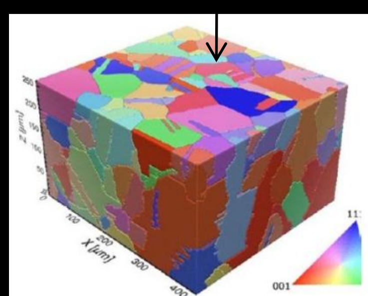
Statistical Homogenization framework

Elasto-ViscoPlasticity Model + Statistical Continuum Mechanics
D. Li (PNNL), H. Garmestani (GT)

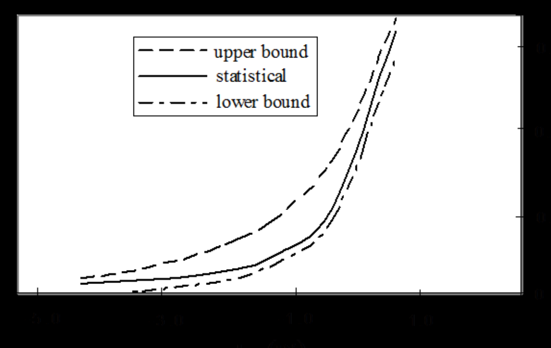
Orientation map with orientations indicated by false colors obtained using Orientation Imaging Microscopy in a scanning electron microscope.



Voronoi tessellated polycrystal model statistically similar to real microstructures.



Reconstruct 3D microstructure from phase field models (PFM) and experimental datasets



Statistical Homogenization
Plastic Property Prediction

Given:

1. Equilibrium $\sigma_{ij,j} = 0$
2. Incompressibility $L_{ii} = 0$

Solve: *v*, *p*

The solution to these set of PDE's are given by Green's function

$$v_i(\mathbf{r}) = \bar{v}_i + \int_{\mathbf{r}' \in V} G_{ij}(\mathbf{r}-\mathbf{r}')F_j(\mathbf{r}')d\mathbf{r}'$$

$$p(\mathbf{r}) = \bar{p} + \int_{\mathbf{r}' \in V} H_i(\mathbf{r}-\mathbf{r}')F_i(\mathbf{r}')d\mathbf{r}'$$

$$F_i = \left[\tilde{N}_{ijkl} L_{kl}\right]_{,j}$$

After obtaining the Green's function solution, the velocity gradient $L_{ij}=v_{i,j}$

$$L_{ik}(r) = \bar{L}_{ik} + \int_{r' \in V} G_{ij,k}(r-r')\left[\tilde{N}_{jlrs}(L(r'),h(r'))L_{rs}(r')\right]_{,l} dr'$$

$$= \bar{L}_{ik} + \int_{r' \in V} G_{ij,kl}(\mathbf{r}-\mathbf{r}')\tilde{N}_{jlrs}(L(\mathbf{r}'),h(\mathbf{r}'))L_{rs}(\mathbf{r}')d\mathbf{r}'$$

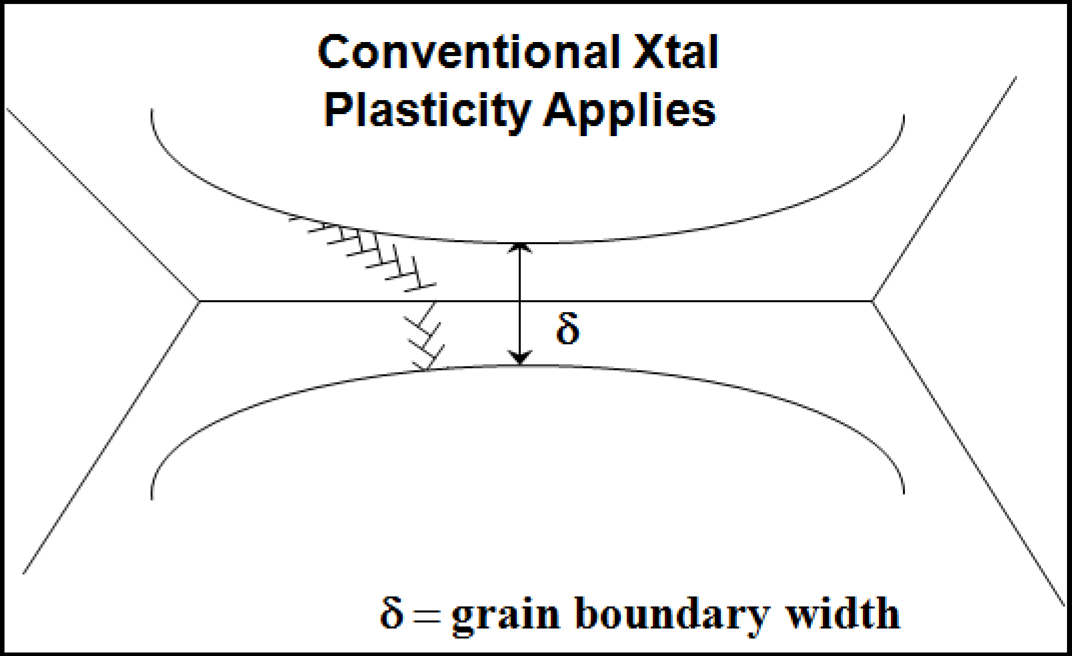
Constitutive equation

$$\mathbf{D} = \frac{\dot{\gamma}_0}{g^\alpha}\sum_\alpha \left(\frac{\mathbf{P}^\alpha \cdot \mathbf{S}}{g^\alpha}\right)^{n-1}(\mathbf{P}^\alpha \otimes \mathbf{P}^\alpha)\cdot\mathbf{S} \equiv \mathbf{M}(\mathbf{S})\cdot\mathbf{S}.$$

$M=N^{-1}$

Deformation at GBs

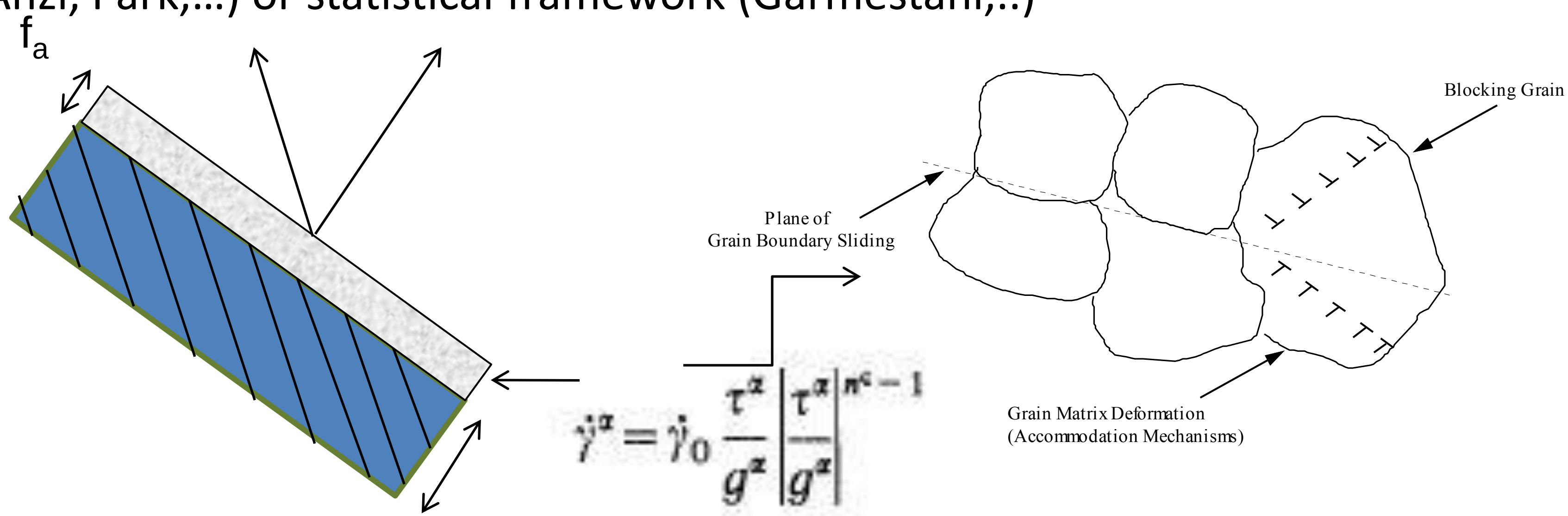
Because of the discontinuity in slip systems and the interactions with deformation activity in neighboring grains, the near grain boundary region responds differently than grain interiors.



In the grain boundary region a boundary specific constitutive law is applied. In the most physical sense the exact structure of each boundary should be known to predict how active slip systems on either side of the boundary interact with each other.

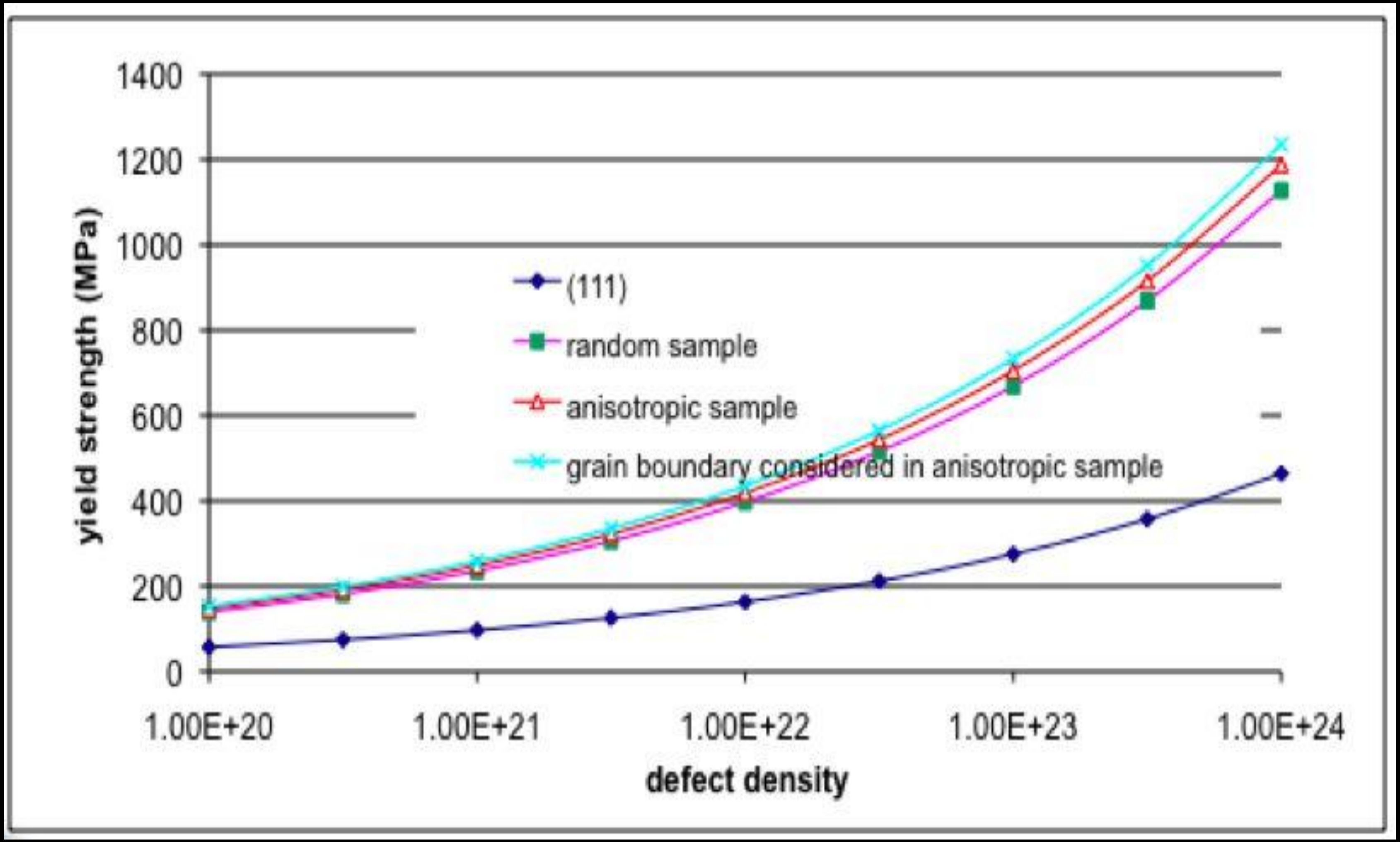
Effect of Grain boundary in Crystal Slip

- Grain Boundaries can be considered as a second phase amorphous regions with special properties.
- The effect of crystal orientation is taken care by the ODF input
- These properties evolve due to radiation and the effect can be taken into account in the grain boundary constitutive equations.
- The effect of hardening is taken care of directly in the crystal plasticity formulation hardening laws.
- The cell can then be homogenized through a self-consistent scheme (S. Ahzi, Park,…) or statistical framework (Garmestani,..)



$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \frac{\tau^{\alpha}}{g^{\alpha}} \left| \frac{\tau^{\alpha}}{g^{\alpha}} \right|^{n^c - 1}$$

Putting it all Together! MD-DD-GB-CP
Effect of Defect Density and grain boundary (a-Fe)



Work in progress:

- Developing Data base for Fe-Ni and Fe-Cr
- Generating input scripts to run further simulations of defect (cavities, helium bubbles), element segregation, and their effect on mechanical properties
- *Developing code for obtaining minimum energy grain boundary structures*
- *Build a database of HT9 grain boundary structures*
- *Develop the computational framework and codes for ascertaining evolution laws at the meso-macor level.*