Engineering Diffraction:
Update and Future Plans

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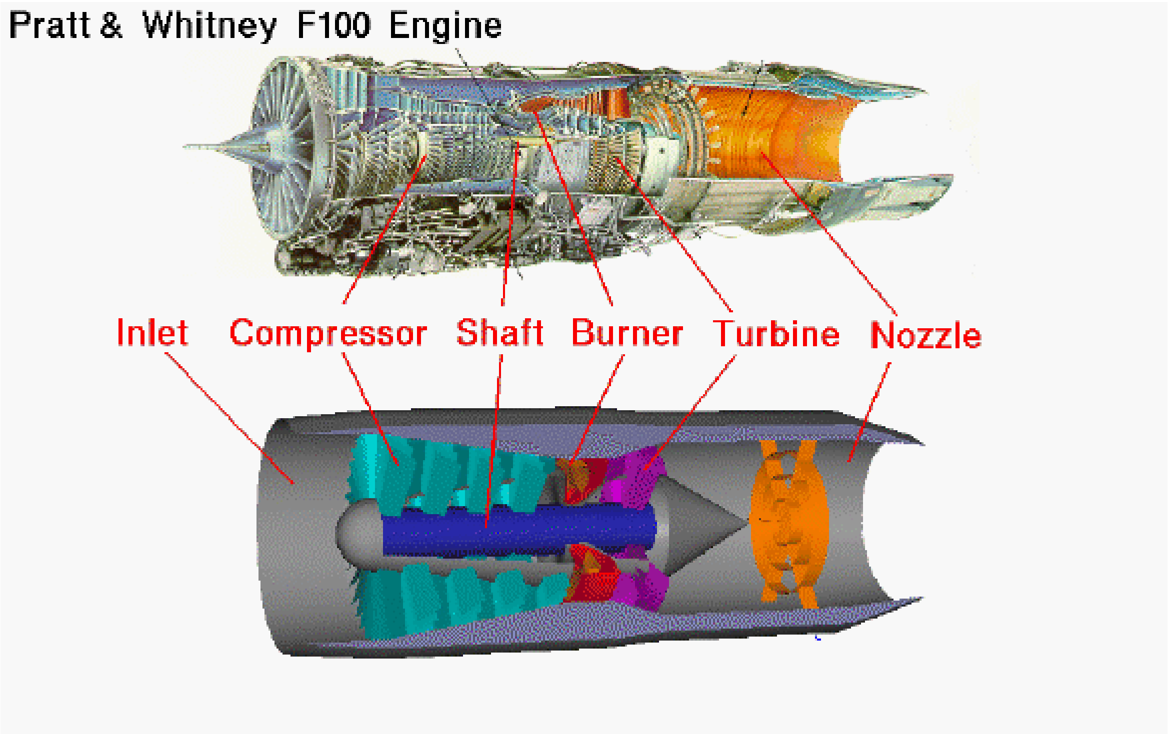
Engineering Diffraction: *Scope*



- <u>Main objective</u>: Predict lifetime and performance
- Needed:
  - Accurate in-situ constitutive laws: $\sigma = f(\varepsilon)$
  - Measurement of service conditions: *residual and internal stress*

Engineering Diffraction: *Typical Experiment*

Typical engineering studies:

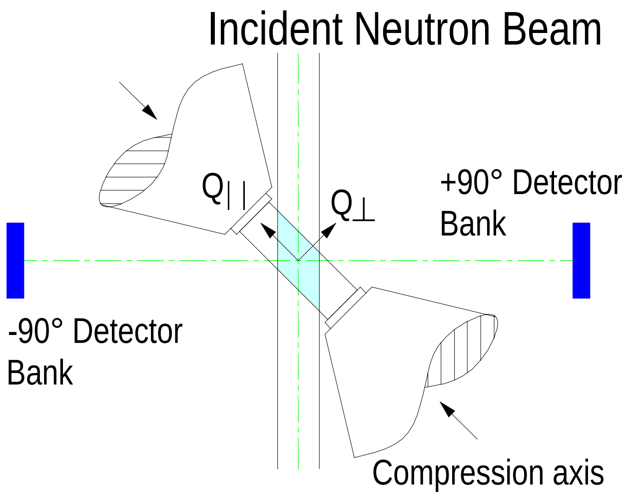
- Deformation studies
- Residual stress mapping
- Texture analysis
- Phase transformations

Eng. Diffractometers:

SMARTS (LANSCE)

ENGIN X (ISIS)

VULCAN (SNS)

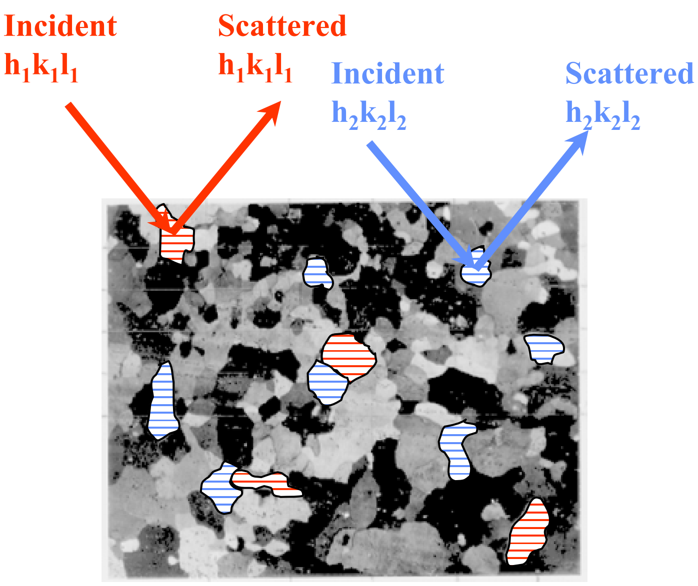


Challenges:

- Small strains (~0.1%)
- Quick and accurate setup
- Efficient experiment design and execution
- Realistic pattern simulation
- Real time data analysis
- Realistic error propagation
- Comparison to mechanics models
- Microstructure simulation

Bragg's law:
$\lambda = 2d\sin\theta$

$$\varepsilon_{hkl}^{el} = \frac{d_{hkl} - d_{hkl}^{0}}{d_{hkl}^{0}} = \frac{d_{hkl}}{d_{hkl}^{0}} - 1$$



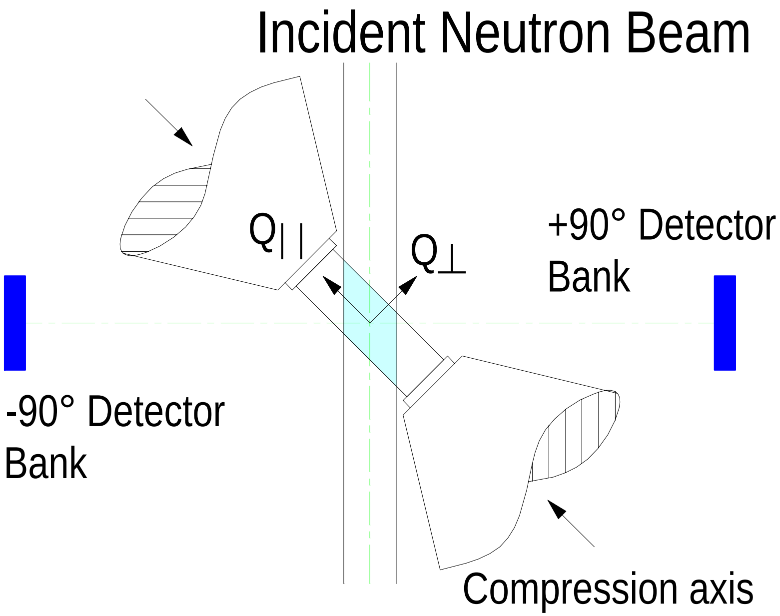
Engineering Diffraction: *Vision for DANSE*

- Objectives:
  - Enable new science (& enhance the value of EngND output)
  - Utilize beam time more efficiently
  - Help enlarge user community

- Approach:
  - Experiment planning and setup: (Task 7.1)
    - Experiment design
    - Optimum sample handling (*SScanSS*)
    - Error analysis
  - Mechanics modeling (*FEA, SCM*): (Task 7.2)
    - Multiscale (*continuum to mesoscale*)
    - Constitutive laws: $\sigma = f(\varepsilon)$
  - Experiment simulation: (Task 7.3)
    - Instrument simulation (*pyre-mcstas*)
    - Microstructure simulation (*forward / inverse analysis*)

- Impact:
  - Re-definition of diffraction stress analysis
  - Easy transfer to synchrotron XRD

Engineering Diffraction: *Typical Experiment*



Proposed Applications

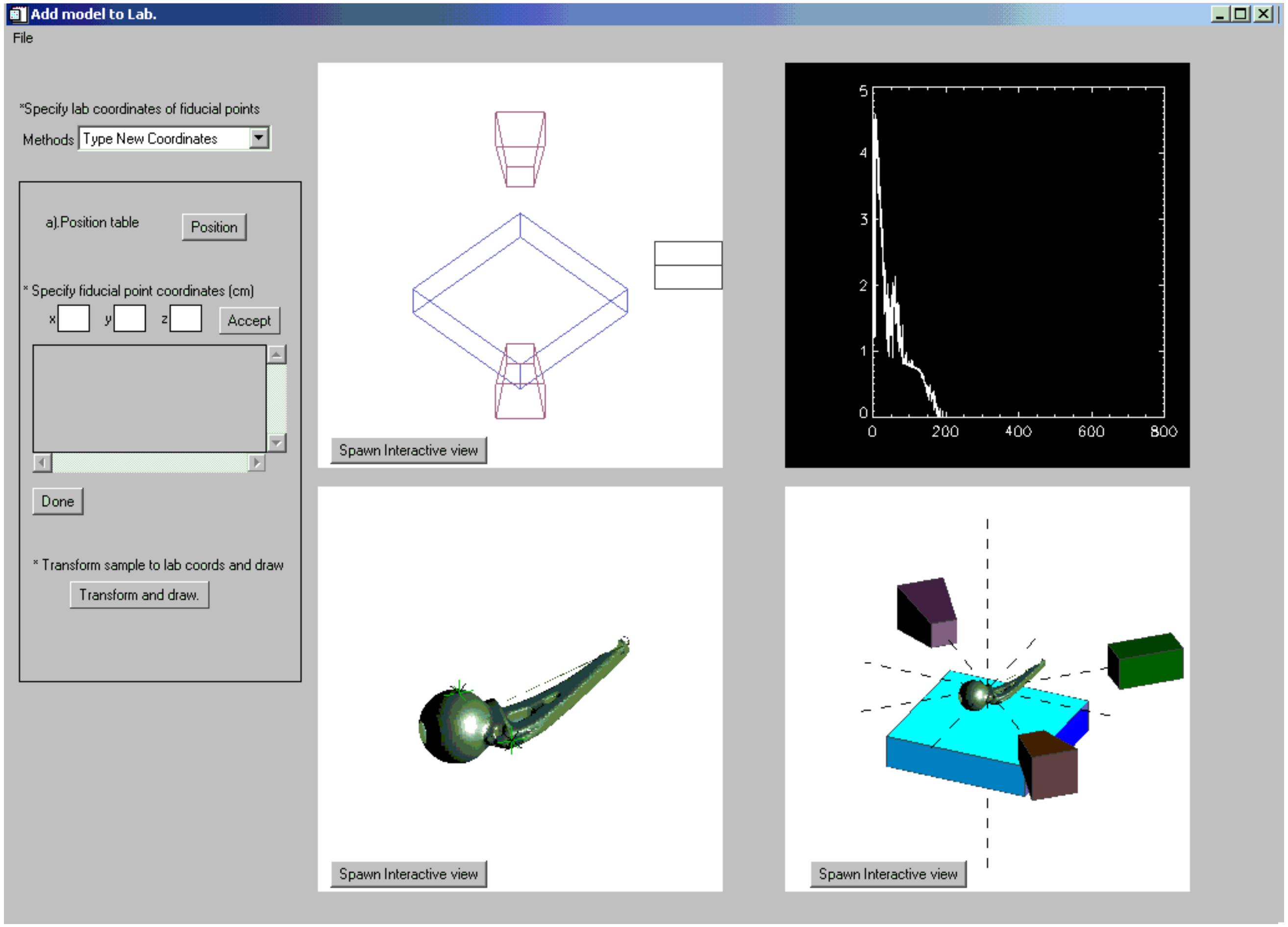
1. Experiment Design and Simulation
   - Instrument simulation
   - Optimization of parameters
   - Microstructure simulation
2. Mechanics modeling I: finite element analysis (FEA)
3. Mechanics modeling II: self-consistent modeling (SCM)
4. Data analysis

Efforts underway in all of these tasks

Experiment Design and Simulation

- **Instrument simulation**
  - ***McStas***
  - **Machine studies (SMARTS, ENGIN X)**
- **Optimization of parameters**
  - **Sample setup and alignment (*SScanSS*)**
  - **Parametric studies (e.g., neural network analysis)**
- **Microstructure simulation**
  - **Defining the sample kernel for experiment simulation**
  - **Full *forward* simulation of experiment**

ISIS: *SScanSS* Software



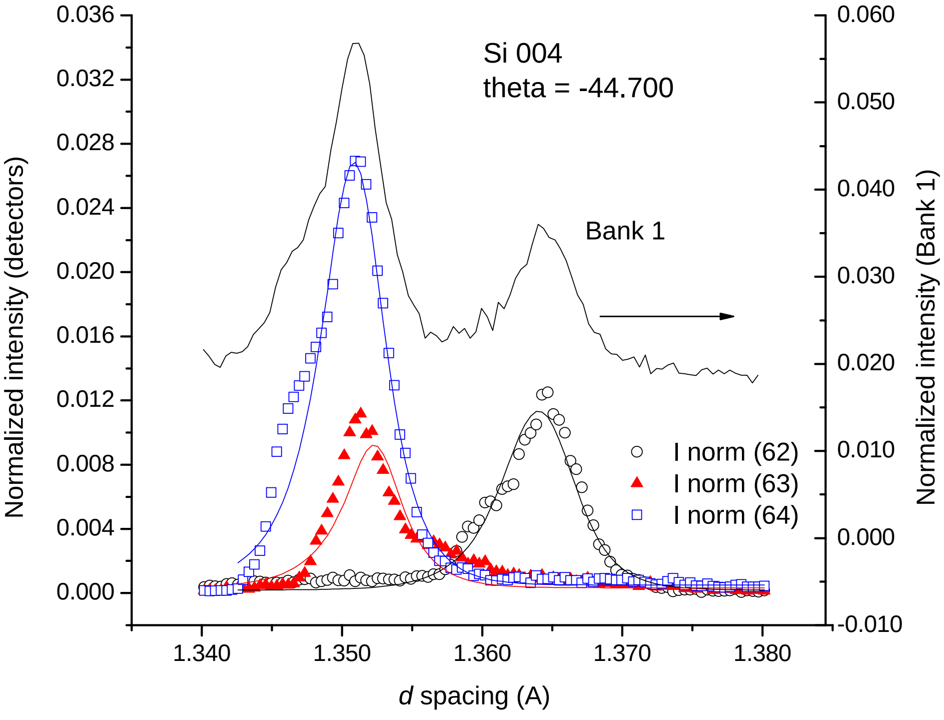
- **Implemented on ENGIN X**
- **Ideal for efficient sample setup**
- **Controlled by IDL scripts**
- **Generates a computer image of sample**
- **Creates and executes a measurement plan**
- **Performs GSAS analysis**
- **Creates 2-D data/result plots**

J. James *et al.*

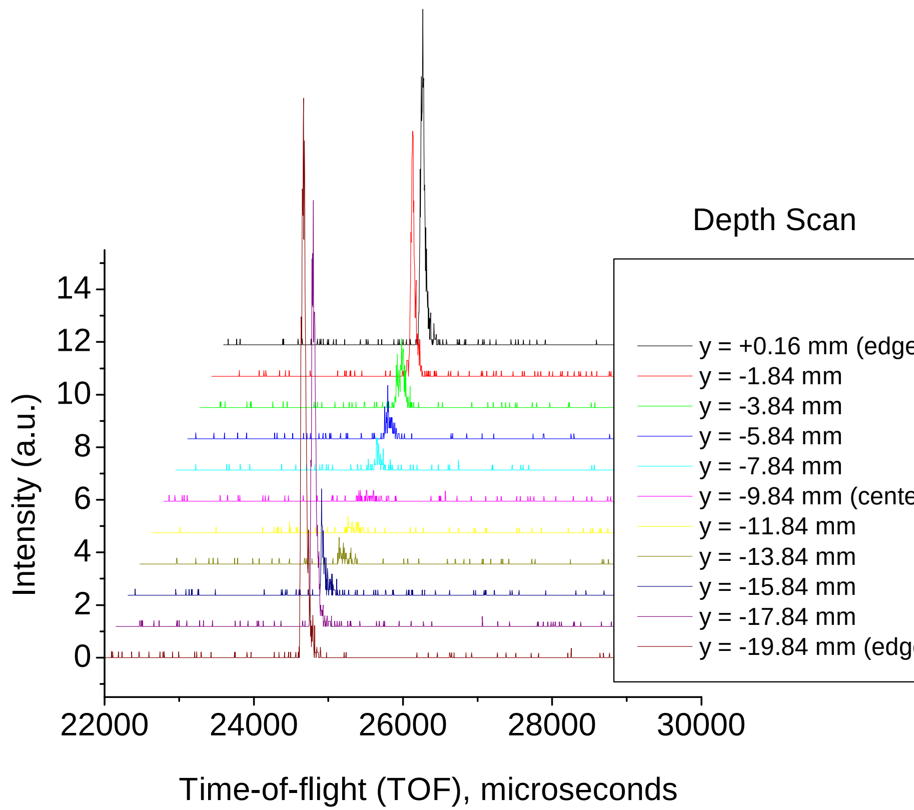
Experiment Design and Simulation

- Instrument characterization (machine studies)

SMARTS

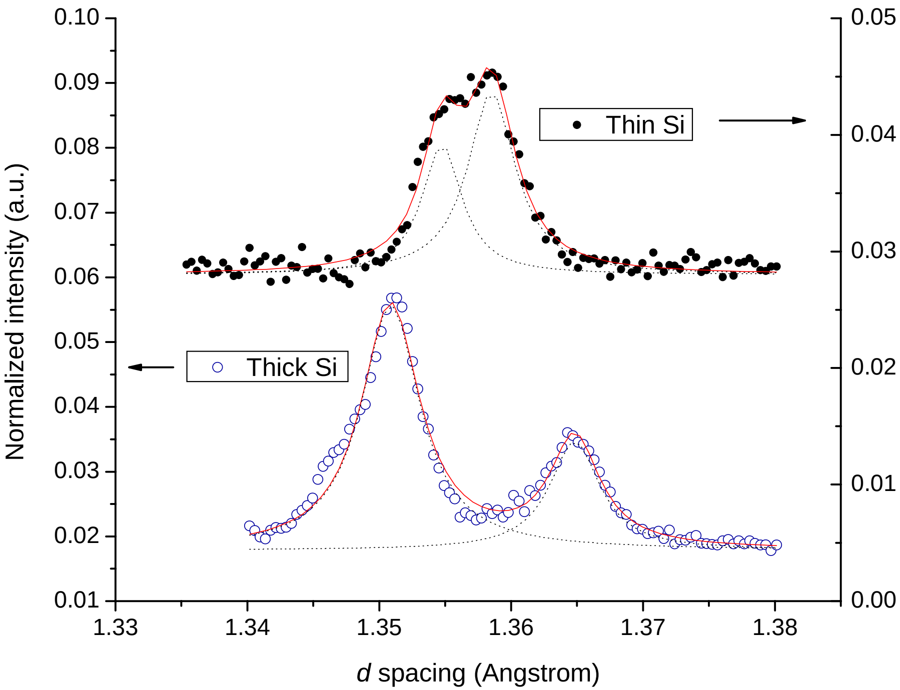


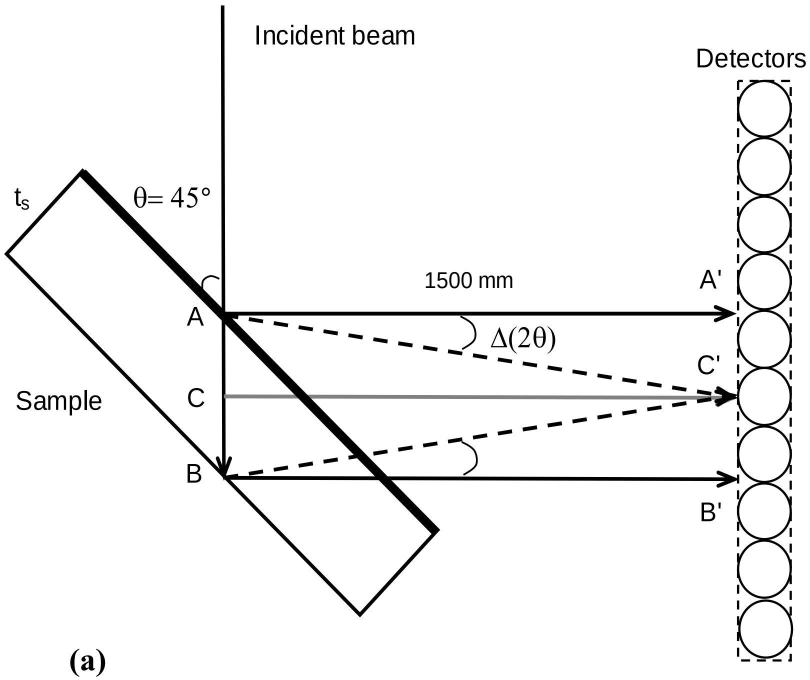
ENGIN-X



Engineering Diffraction: *Microstructure*

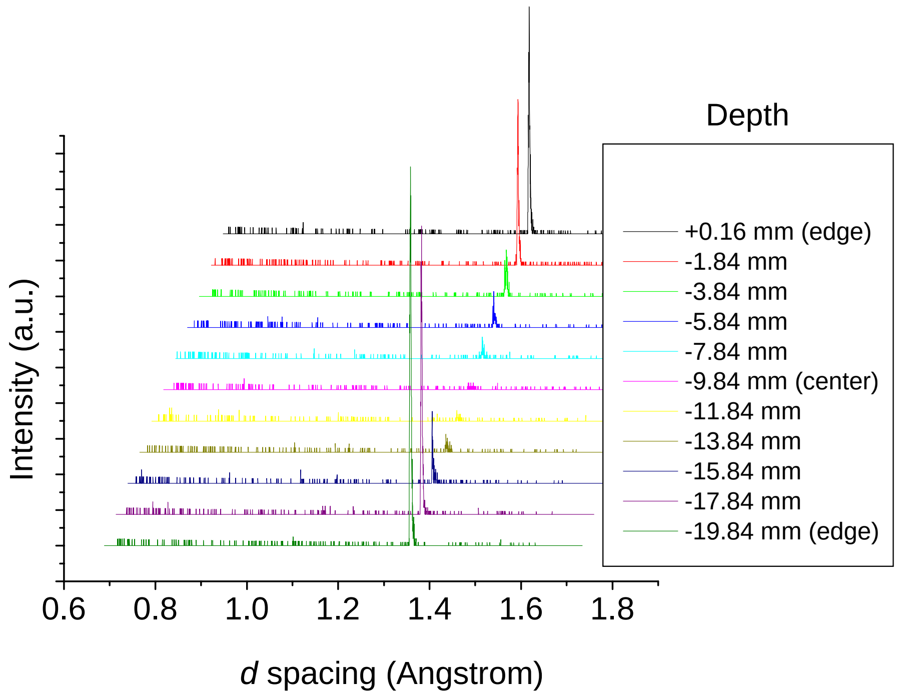
- Si single crystals (0.7 and 20 mm thick)
- SMARTS data
- Double peaks due to dynamical diffraction

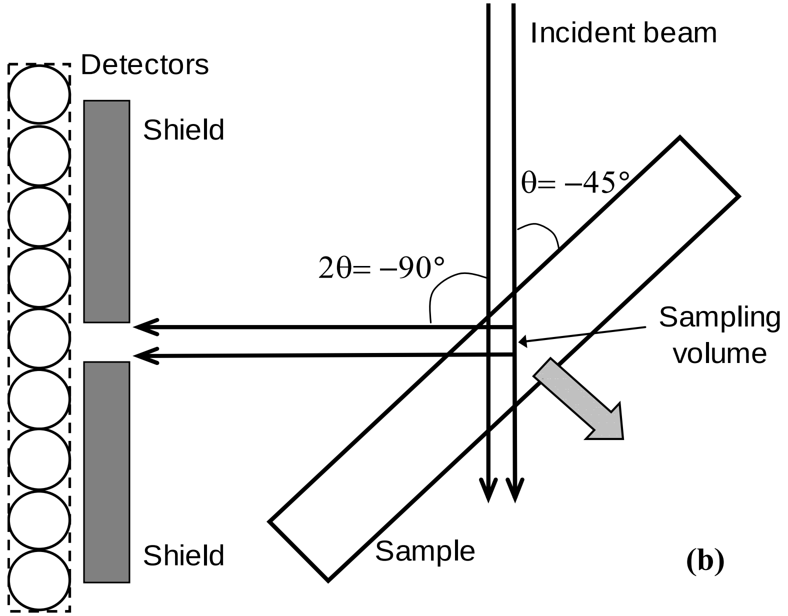




Engineering Diffraction: *Microstructure*

- Si single crystal (20 mm thick)
- ENGIN-X depth scan
- Data originates from surface layers



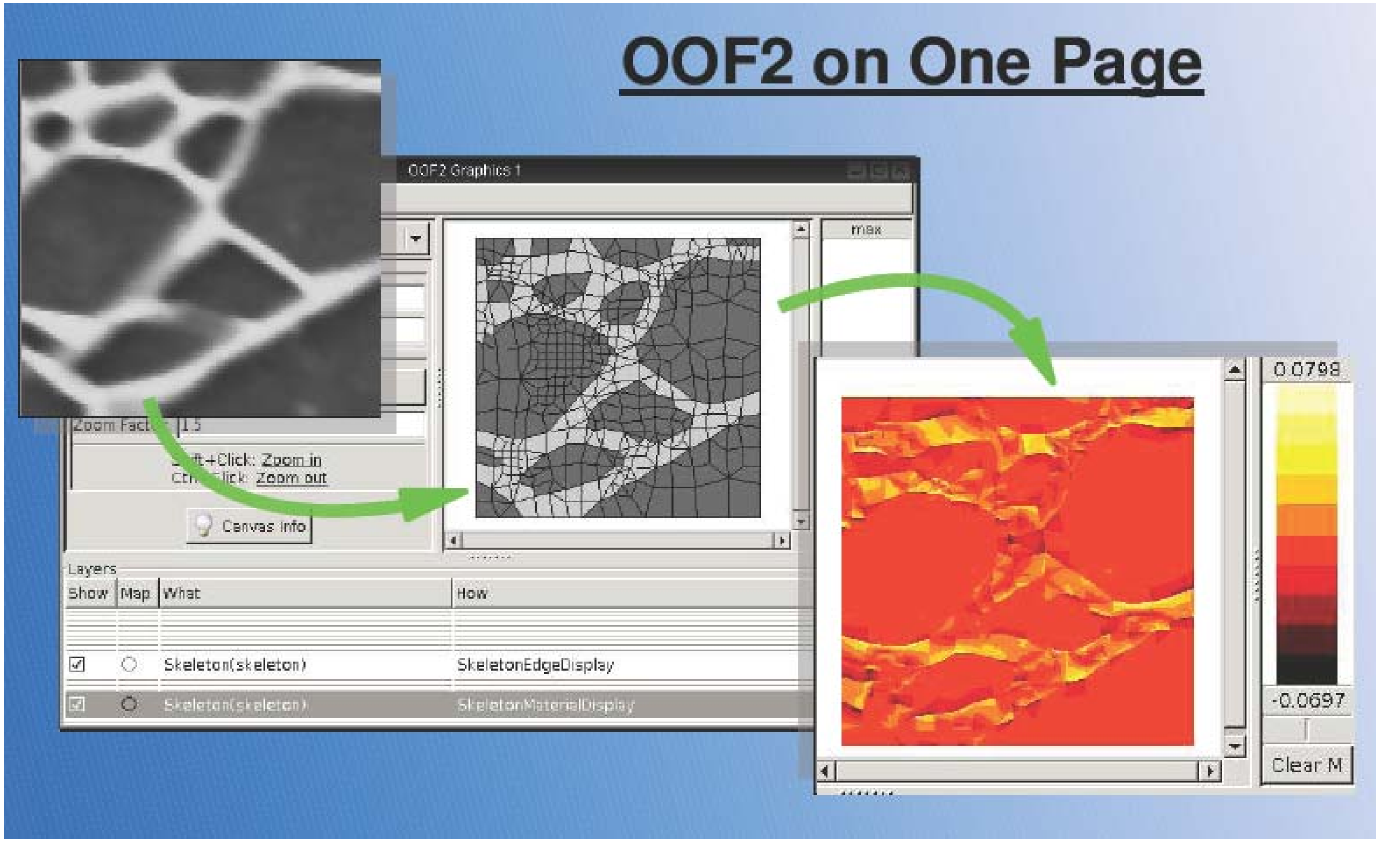


<u>Critical question</u>: *Transition between a single crystal and polycrystal?*

E. Ustundag *et al.*, Appl. Phys. Lett. (2006)

Object Oriented Finite Element Analysis

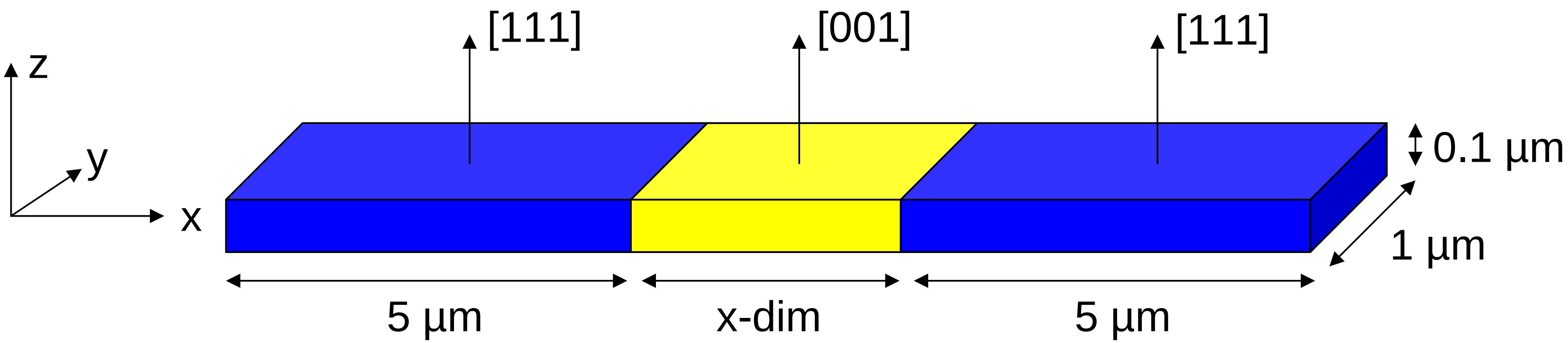
- Modeling of real microstructure
- Will be employed in DANSE for microstructure modeling
- Needs to become 3-D and validated



A. Reid (NIST)

Microstructure Simulation

Three Grain Model Description



- **Unixaxial Tension:**

  $\sigma_{applied}$ = 100, 200 & 300 MPa (along x)

- **x-dim varies:**

  5 µm, 3 µm, 1 µm, 0.8 µm, 0.6 µm

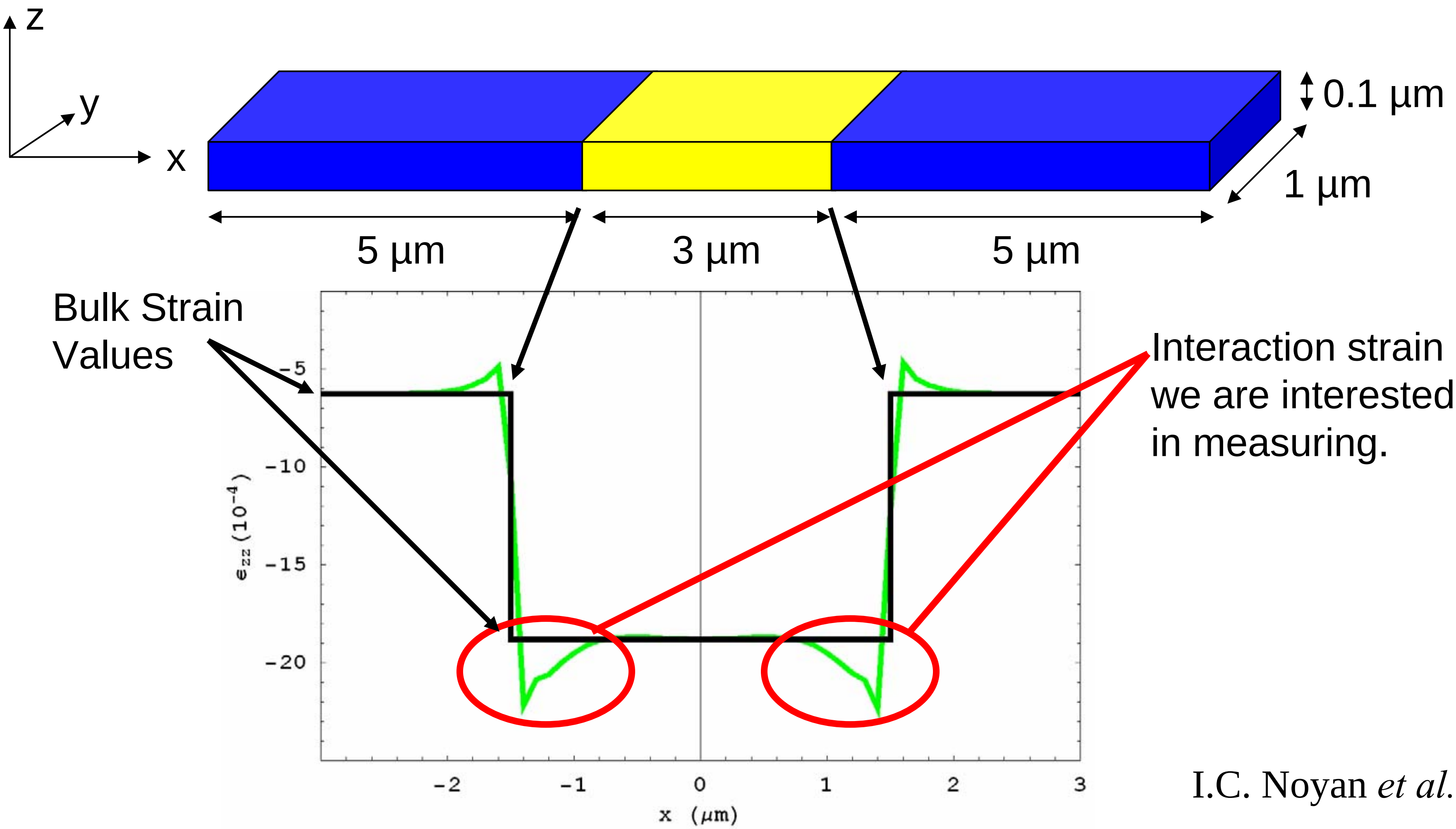
- **Cu parameters**

  C^{111}_{11} = 220.3 GPa, C^{111}_{12} = 104.1 GPa, C^{111}_{44} = 40.8 GPa
  C^{001}_{11} = 168.4 GPa, C^{001}_{12} = 121.4 GPa, C^{001}_{44} = 75.4 GPa

I.C. Noyan *et al.*

Results from FE Model (300 MPa)

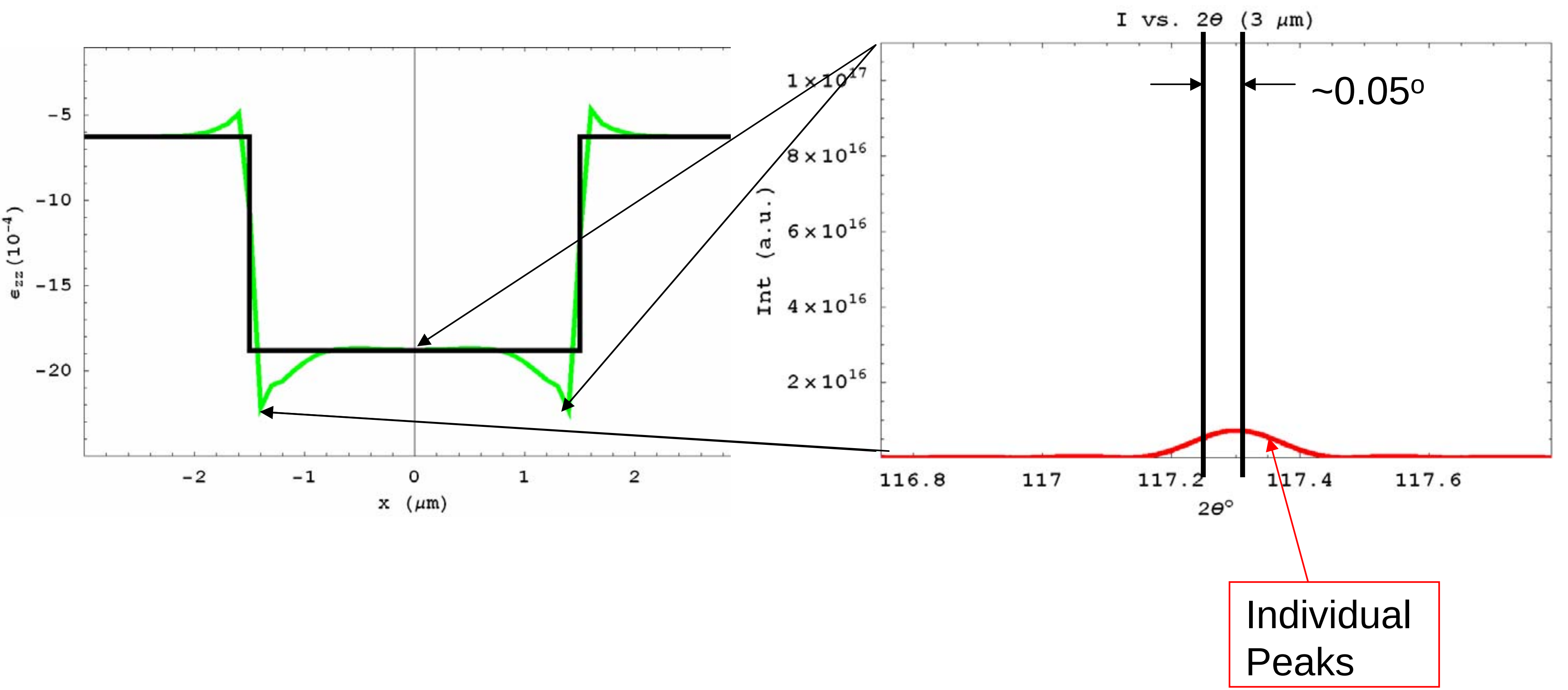
- **Using COMSOL Multiphysics, we obtain the out of plane strain along center line in central grain.**



I.C. Noyan *et al.*

Kinematic X-Ray Modeling

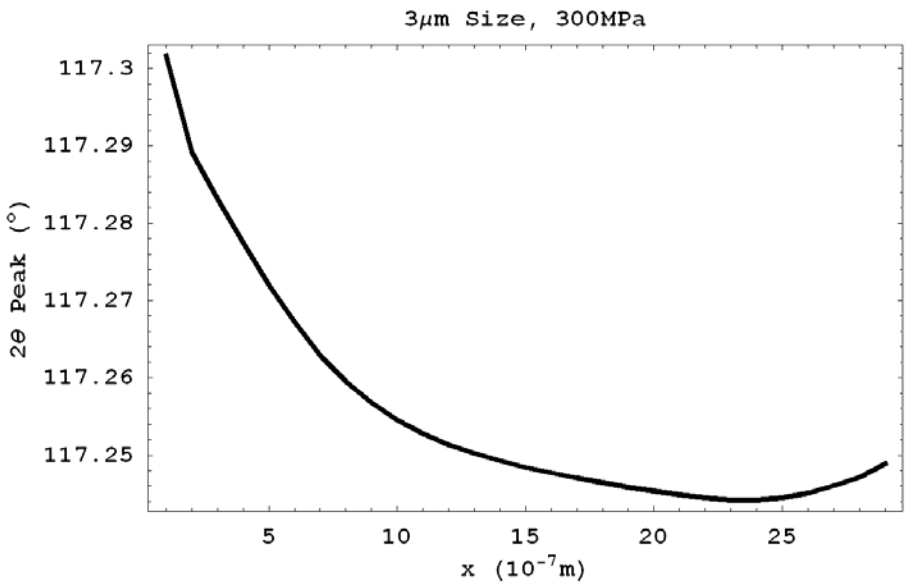
- **Using kinematic diffraction theory, we simulate a rocking curve diffraction pattern.**

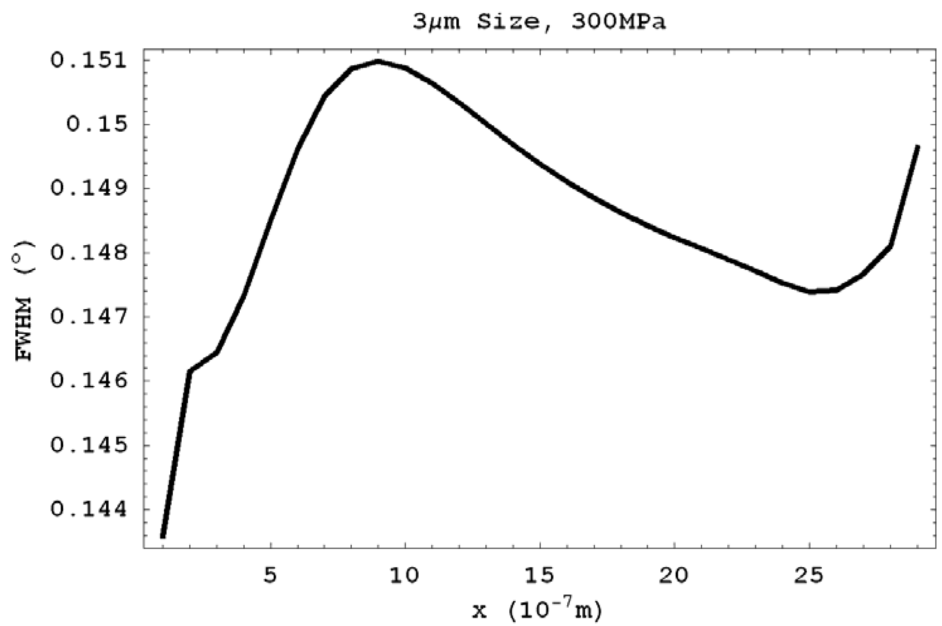


I.C. Noyan *et al.*

Peak Fitting Analysis

- **Fitting the diffraction peak with multiple Gaussians, it is possible to determine the peak position and breadth at each step of the summation.**





- *How to determine strain profiles from peak position and shape?*
- *What happens in the inelastic regime?*

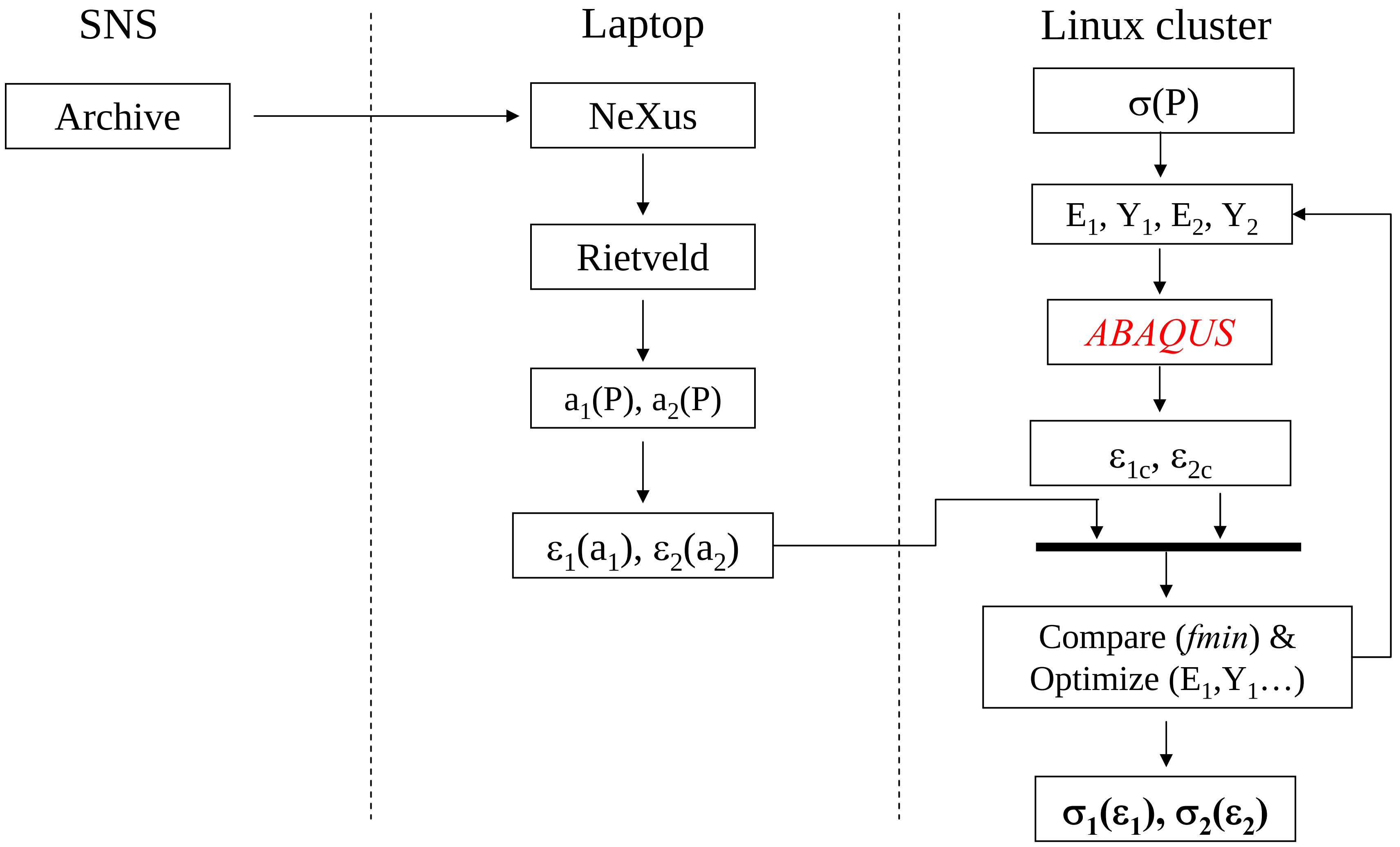
I.C. Noyan *et al.*

Mechanics Modeling

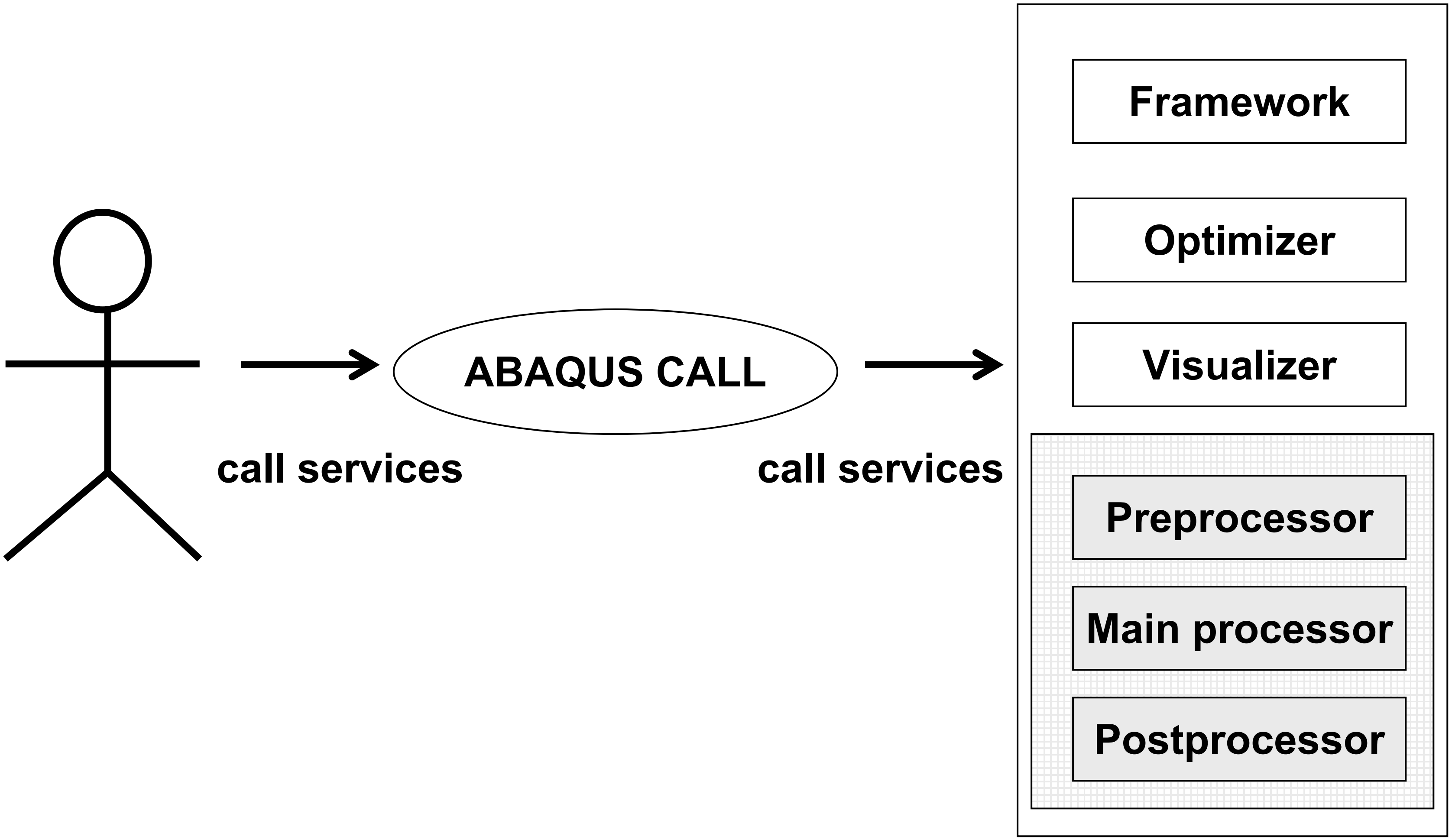
- **Finite element analysis (FEA)**
  - ***ABAQUS***
  - **Optimization of material parameters**

- **Self-consistent modeling (SCM)**
  - ***EPSC* code from LANL**
  - **Optimization of material parameters**

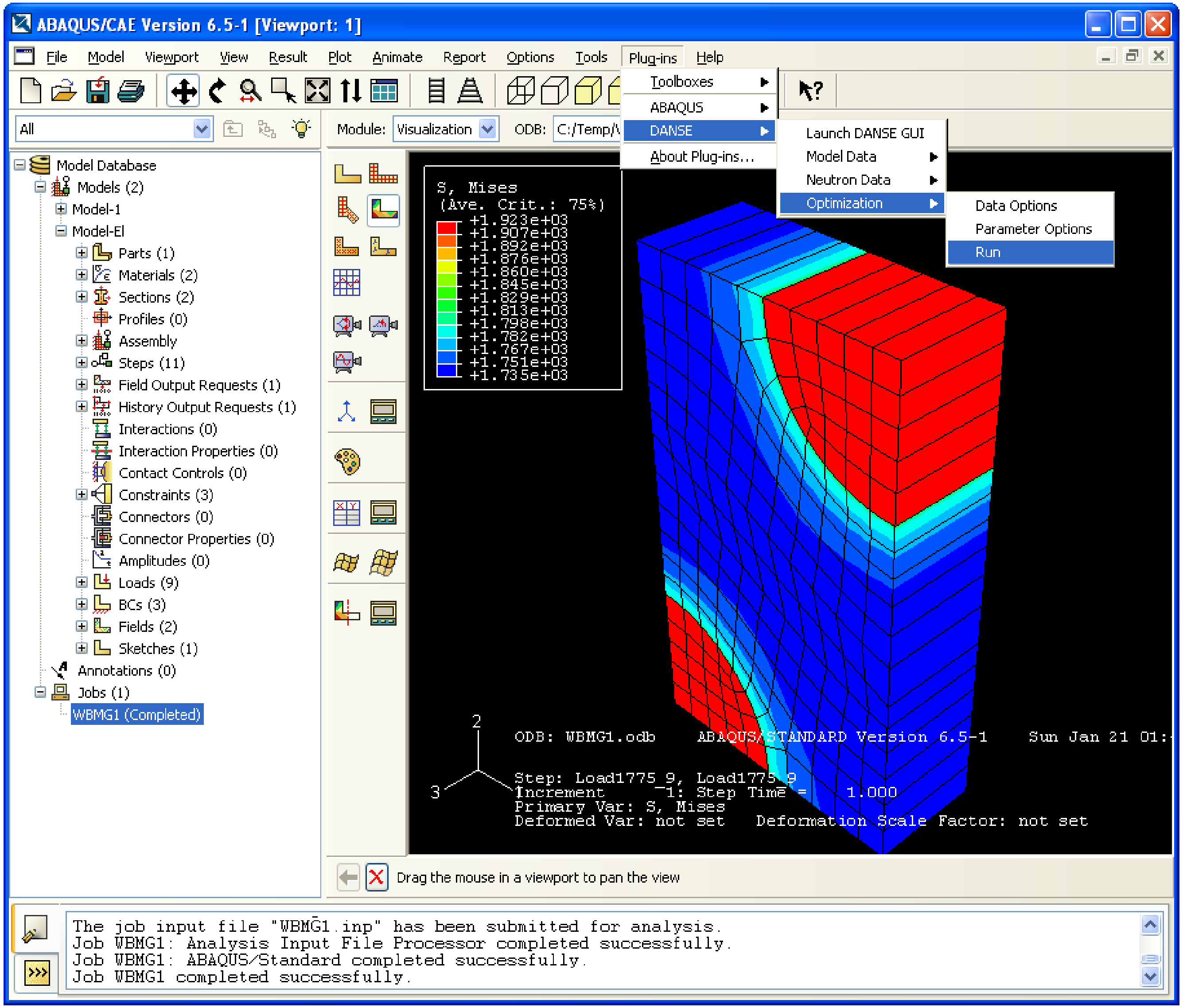
Mechanics Modeling: *FEA* (Finite Element Analysis)



Use Case Diagram for FEA Application

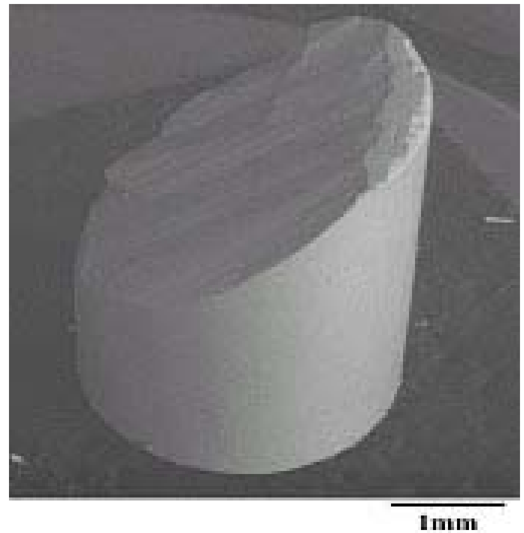


FEA (Finite Element Analysis)

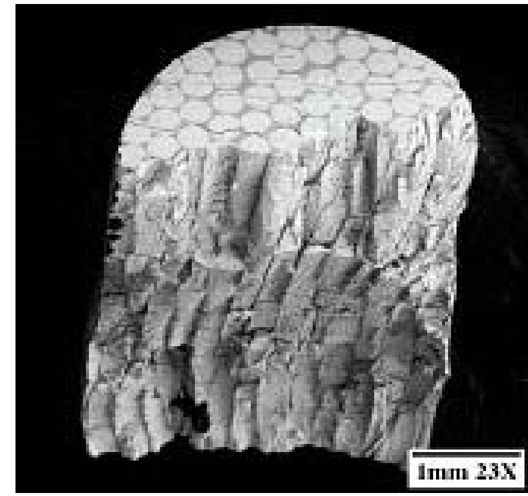


Example: *BMG-W fiber composite*

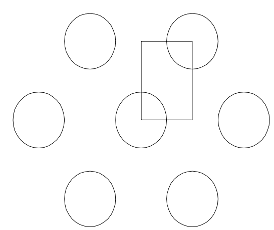
- **Residual stresses**
- **Compression loading at SMARTS**
- **Experiments on 20% to 80% volume fraction of W**
- **Unit cell finite element model**
- **GSAS output for average elastic strain in W in the longitudinal direction**



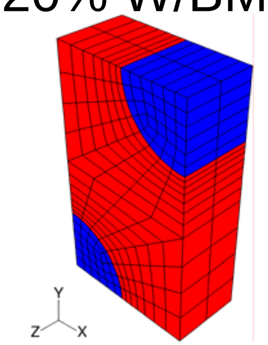
BMG



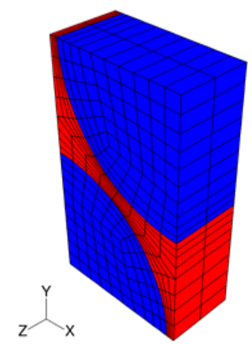
W-BMG composite



20% W/BMG

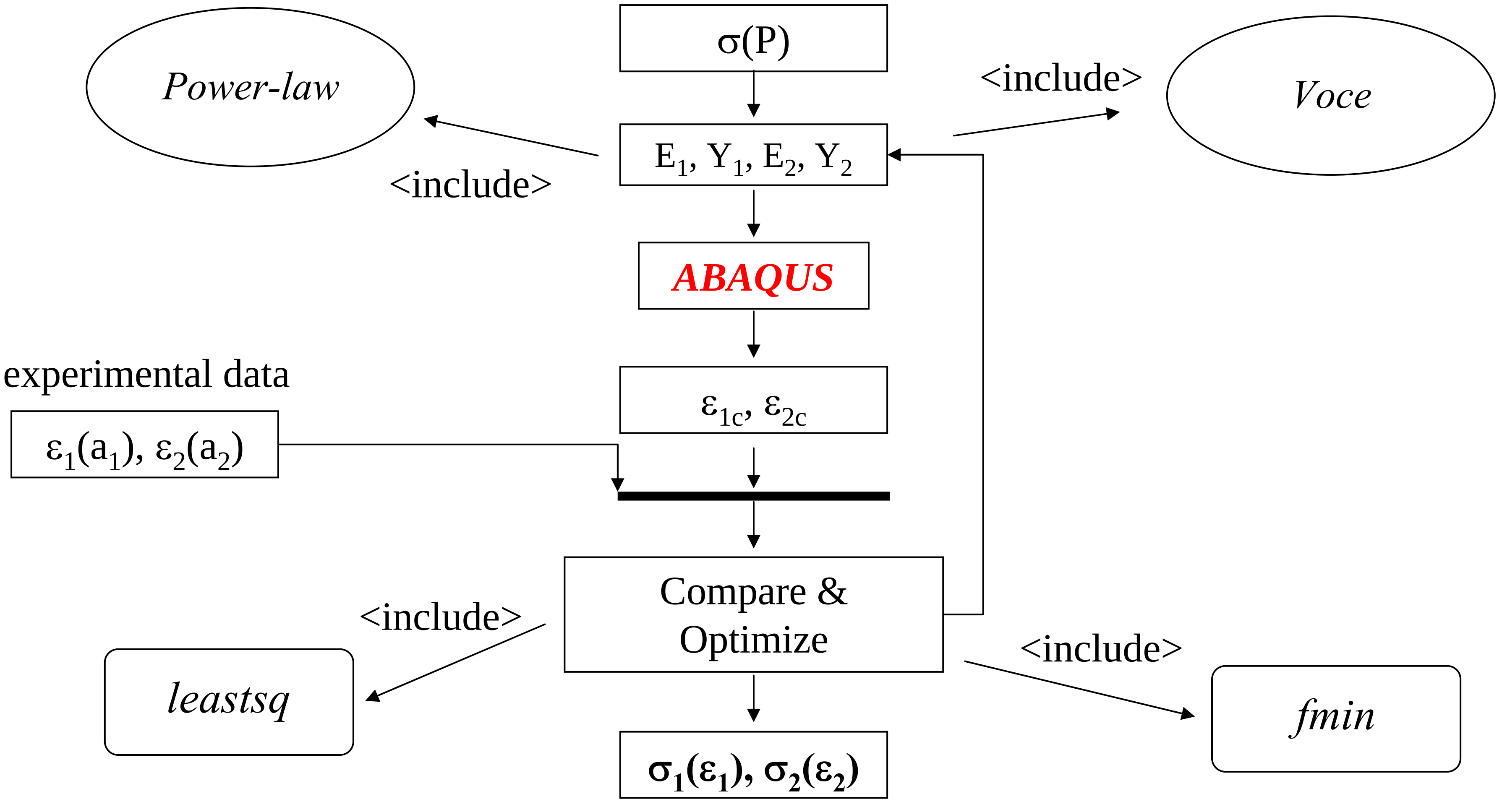


80% W/BMG



Reference: B. Clausen et al., Scripta Mater. 49 (2003) p. 123

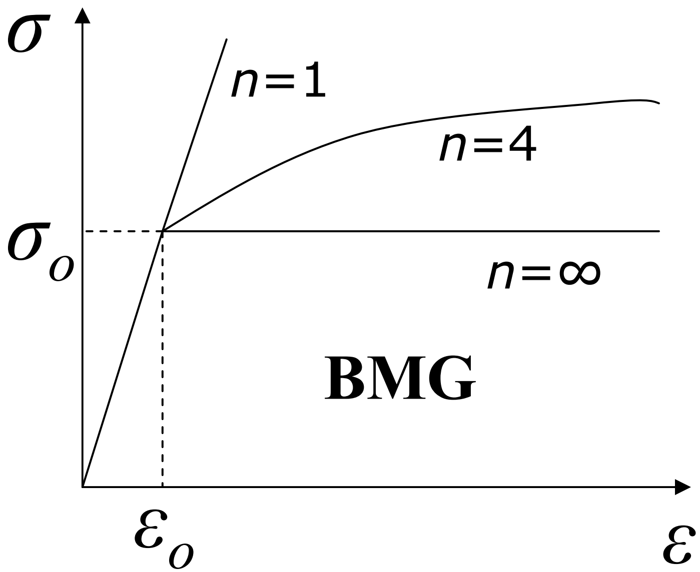
Activity Diagram: *FEA* (Finite Element Analysis)



Easy utilization of various software components

Constitutive Laws for W and BMG

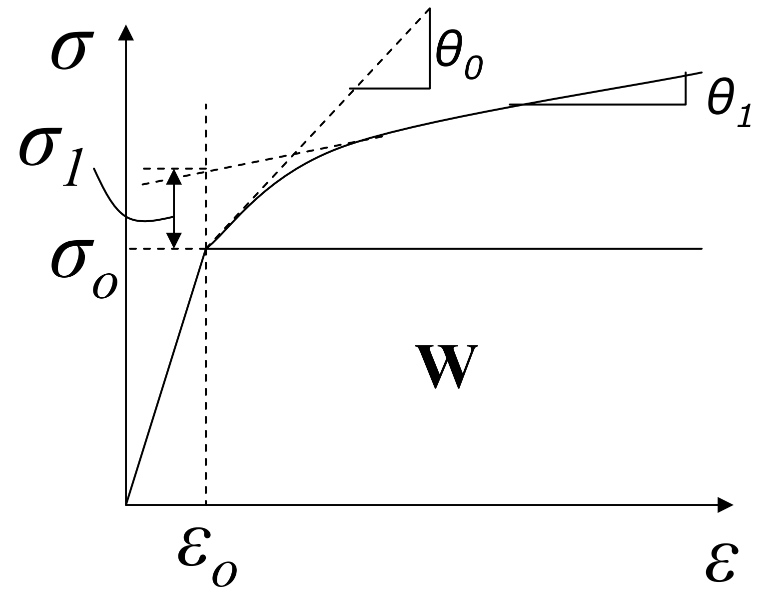
Power-law



$$\frac{\varepsilon}{\varepsilon_o} = \frac{\sigma}{\sigma_o} \quad for\ \sigma \le \sigma_o$$

$$\frac{\varepsilon}{\varepsilon_o} = \left(\frac{\sigma}{\sigma_o}\right)^n \quad for\ \sigma > \sigma_o$$

Voce

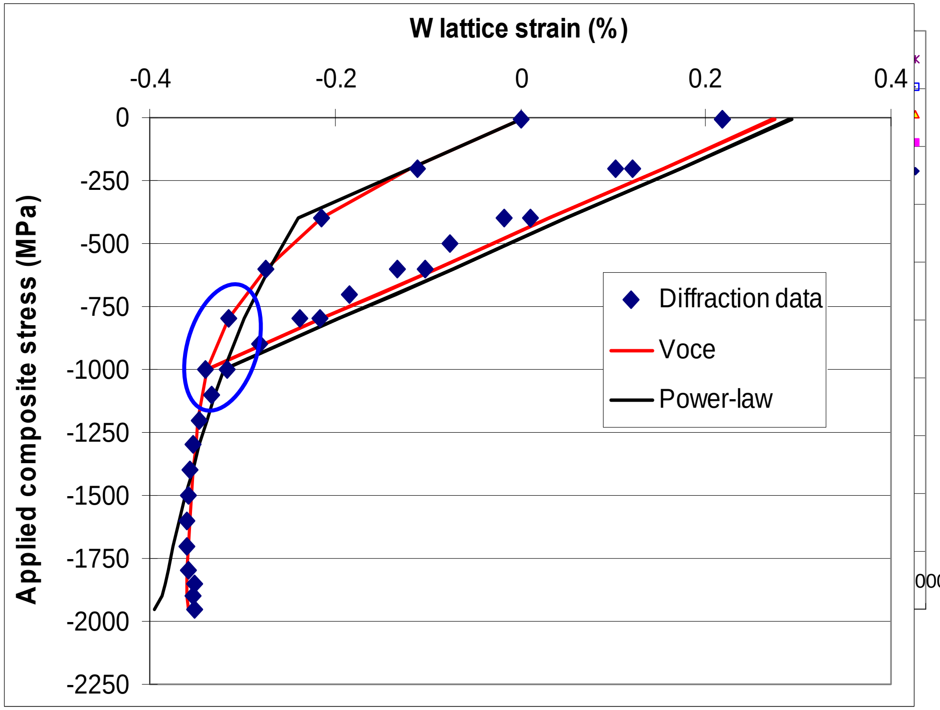


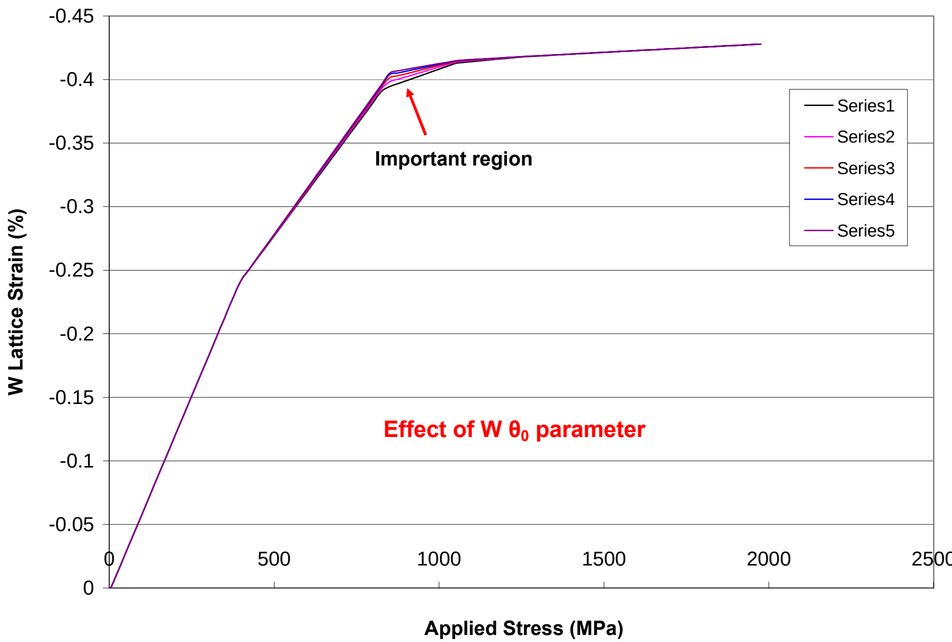
$$\sigma = \sigma_0 + (\sigma_1 + \theta_1 \varepsilon)\left(1 - \exp\left(-\frac{\theta_0 \varepsilon}{\sigma_1}\right)\right)$$

Input parameters: $(\sigma_0)_{BMG}$, n_{BMG}, $(\sigma_0)_W$, $(\sigma_1)_W$, $(\theta_0)_W$, $(\theta_1)_W$ and ΔT

Neural Network Analysis

Sensitivity Studies





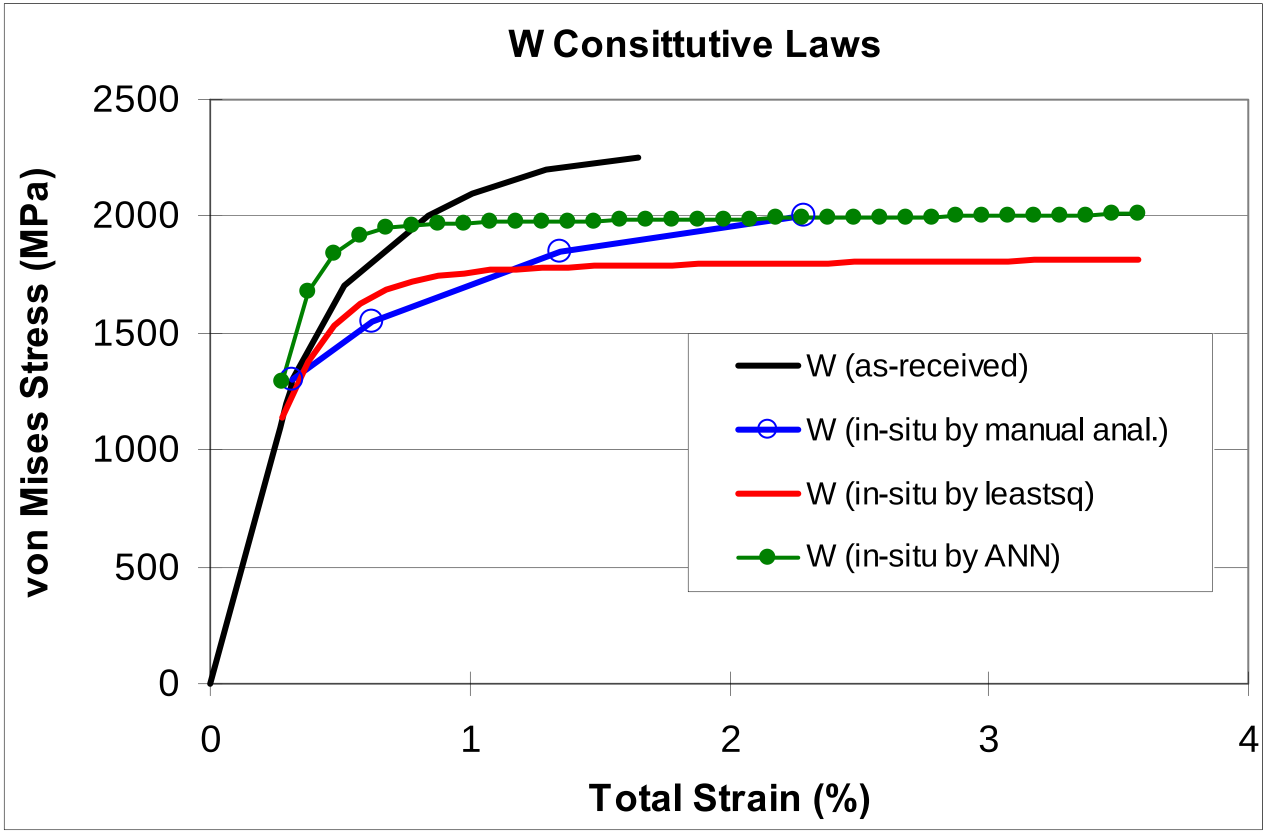
- **Strong influence by parameters: $(\sigma_0)_{BMG}$, $(\sigma_0)_W$, $(\sigma_1)_W$ and $(\theta_0)_W$**
- **Weak/no influence by parameters: n_{BMG}, $(\theta_1)_W$ and ΔT**
- ***Rigorous experiment planning to optimize data collection***

L. Li *et al.*

Neural Network Analysis

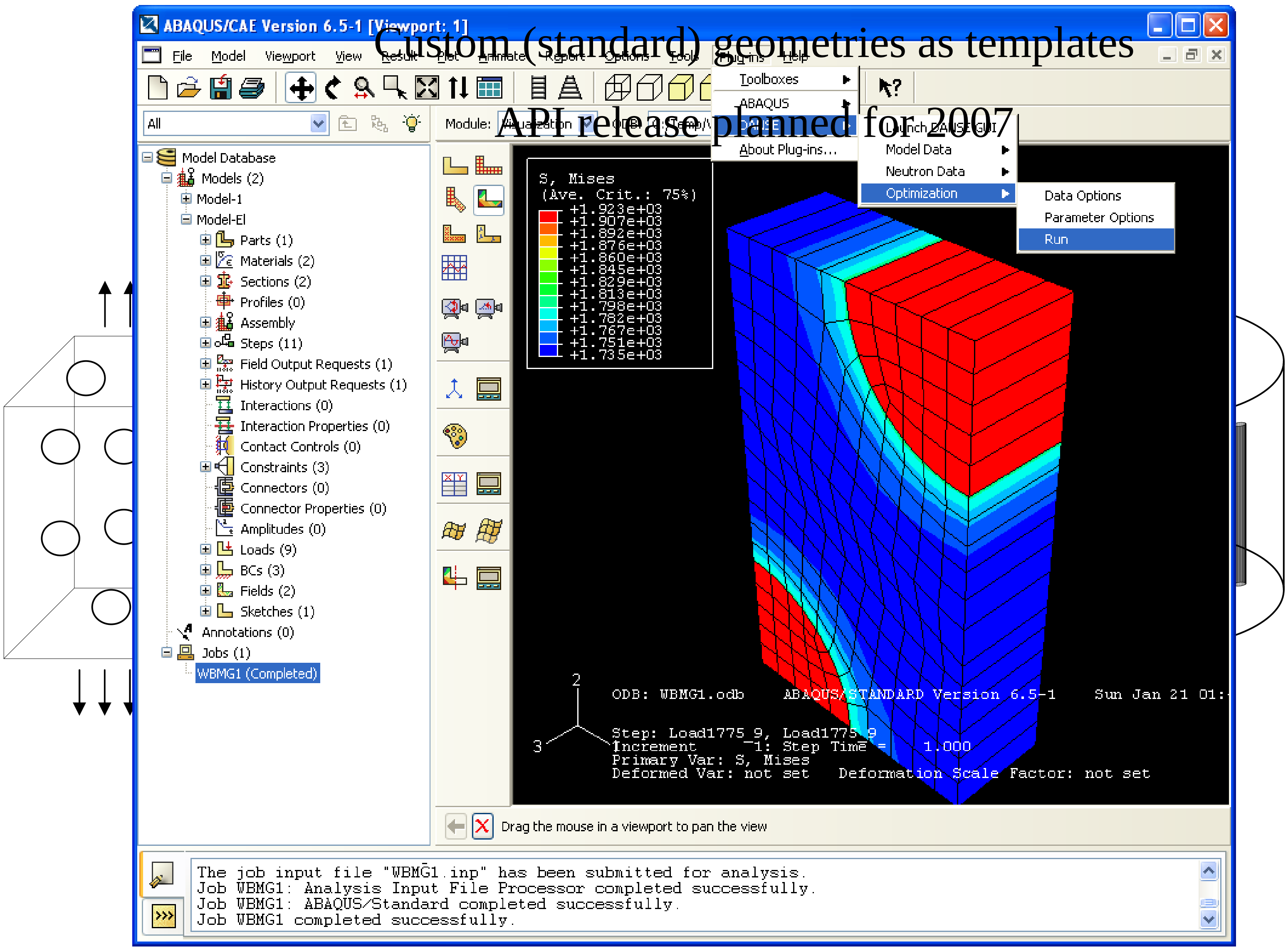
Result

- Use of experimental data for inverse analysis
- Prediction of 'optimum' values of *all 7* input parameters
- Previous analyses optimized only 3 parameters



L. Li *et al.*

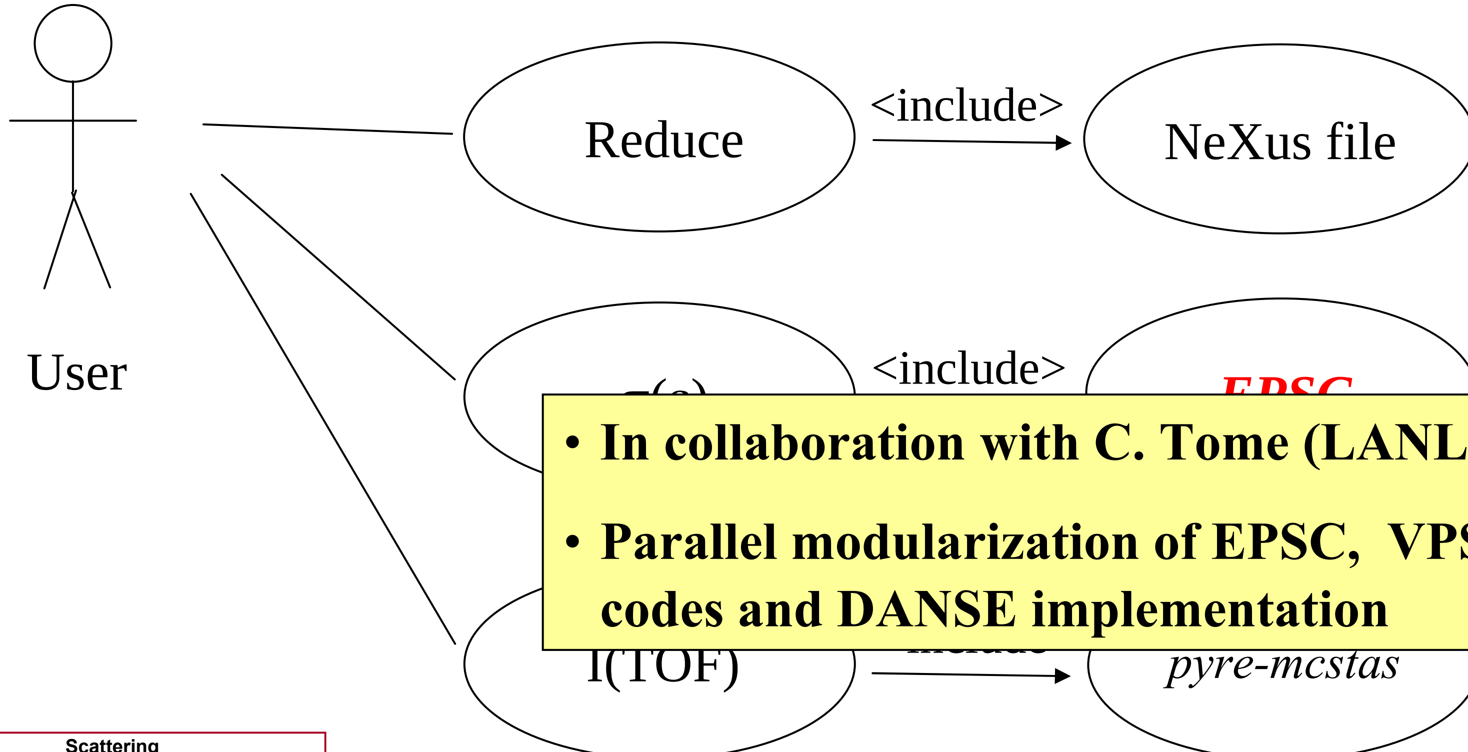
FEA (Finite Element Analysis)



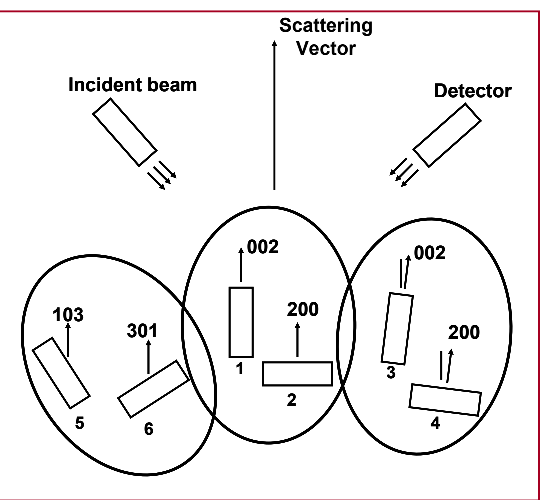
Custom (standard) geometries as templates

API release planned for 2007

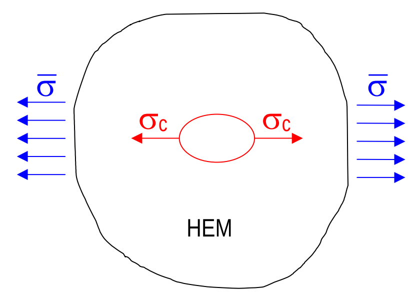
Mechanics Modeling: *Self-Consistent Model*



- **In collaboration with C. Tome (LANL)**
- **Parallel modularization of EPSC, VPSC codes and DANSE implementation**



- Self-consistent modeling (SCM)
- Estimate of lattice strain (*hkl* dependent)
- Study of deformation mechanisms

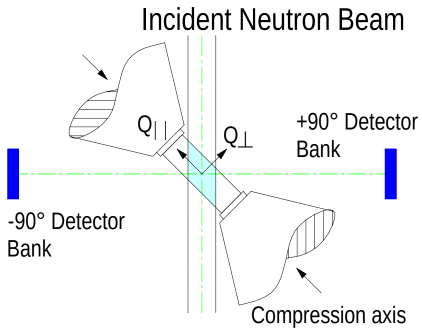


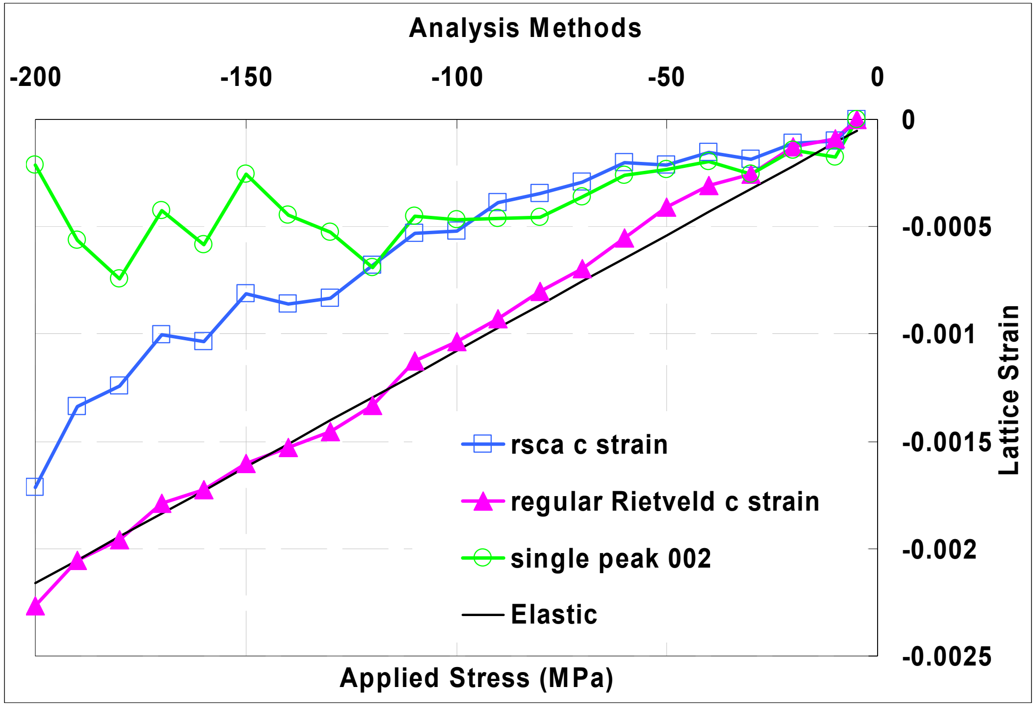
Data Analysis

- **Peak fitting**
  - **Rietveld (full-pattern) analysis *GSAS, DiffLab***
  - **Single peak fitting**
- **Integration of mechanics models to peak fitting**
  - **Strain anisotropy analysis**
- **Texture analysis and visualization *(MAUD)***
- **Real-time data analysis**

Data Analysis: Mechanical Loading of $BaTiO_3$

- Time-of-flight neutron diffraction data from ISIS
- Complete diffraction patterns in one setting
- Simultaneous measurement of two strain directions





M. Motahari *et al.* 2006

Different data analysis approaches:

- Single peak fitting: natural candidate; but some peaks vanish as the corresponding domain is depleted
- Rietveld: crystallographic model fit to all peaks; but results are ambiguous
- Constrained Rietveld: multi-peak fitting, but accounting for strain anisotropy *(rsca);* most promising

Strain Anisotropy Analysis

- Desirable to perform multi-peak fitting (e.g. via Rietveld analysis) to improve counting statistics.
- Question: How to account for strain anisotropy (*hkl*-dependent) due to elastic constants and inelastic deformation (e.g., domain switching)?
- Current approach for *cubic* crystals (in GSAS):

$$\frac{1}{E_{hkl}} = \underbrace{S_{11}}_{Isotropic} - \underbrace{2(S_{11} - S_{12} - S_{44}/2)A_{hkl}}_{Anisotropic}$$

$$A_{hkl} = (h^2k^2 + k^2l^2 + l^2h^2)/(h^2 + k^2 + l^2)^2$$

$$\varepsilon_{hkl} = \underbrace{\frac{d_{hkl} - d^0_{hkl}}{d^0_{hkl}}}_{Isotropic} - \underbrace{\gamma A_{hkl}}_{Anisotropic}$$

Integration of crystallographic and mechanics models

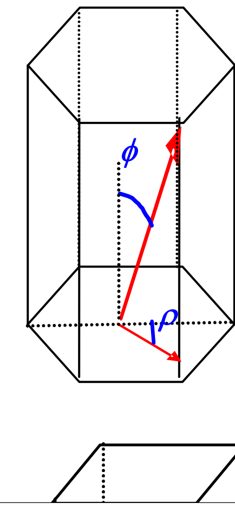
- γ is called 'rsca' and is a refined parameter for some peak profiles.
- Works reasonably well in the elastic regime, but not beyond.
- Needed: rigorous multi-peak fitting with peak weighting and peak shift dictated by mechanics modeling.

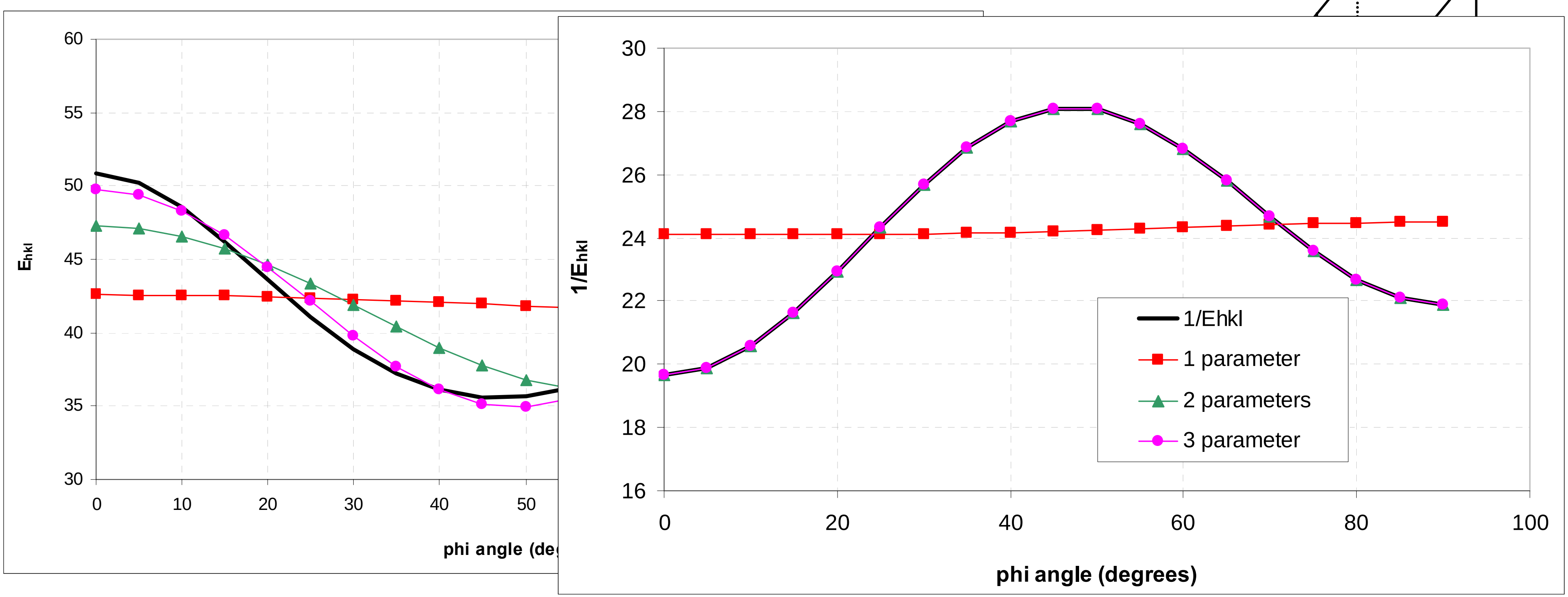
Anisotropic Strain Analysis in Rietveld

$$\frac{1}{E_{hkl}} = (1-l_3^2)^2 S_{11} + l_3^4 S_{33} + l_3^2(1-l_3^2)(2S_{13}+S_{44})$$

$$\varepsilon_{hkl} = \varepsilon_{isotropic} - \gamma \cos\phi$$

$$\varepsilon_{hkl} = \varepsilon_{isotropic} - \gamma_1(1-l_3^2)^2 - \gamma_2 l_3^4 - \gamma_3 l_3^2(1-l_3^2)$$





Engineering Diffraction: *Team*

- E. Üstündag‡, S. Y. Lee, S. M. Motahari, G. Tutuncu (ISU)
- X. L. Wang‡ (SNS) - *VULCAN*
- C. Noyan‡, L. Li, A. Ying (Columbia) – *microstructure*
- M. Daymond‡ (Queens U., ISIS) – *ENGIN X, SCM*
- L. Edwards‡ and J. James (Open U., U.K.) - *SScanSS*
- C. Aydiner, B. Clausen‡, D. Brown, M. Bourke (LANSCE) - *SMARTS*
- J. Richardson‡ (IPNS)
- P. Dawson (Cornell) – *3-D FEA*
- H. Ceylan (ISU) - *optimization*

‡ Member of EngND Executive Committee