Engineering Diffraction:
Update and Future Plans

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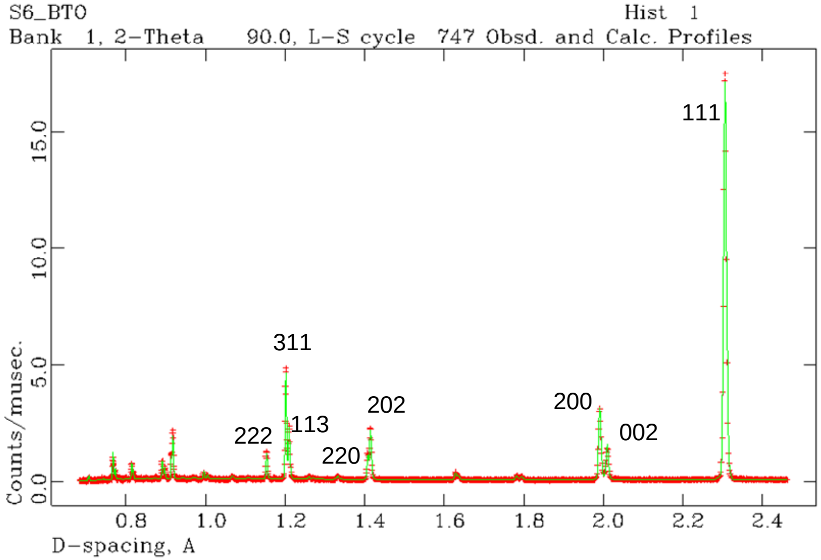
Engineering Diffraction: *Scope*

- <u>Main objective</u>: Predict lifetime and performance
- Needed:
  - Accurate in-situ constitutive laws: $\sigma = f_1(\varepsilon, t, T, a_{O2},\ldots)$
  - Measurement of service conditions: *residual and internal stress*

- <u>Approach</u>:
  - Measure diffraction pattern: d_{hkl}
  - Calculate lattice strain: $$\varepsilon_{hkl}^{el} = \frac{d_{hkl} - d_{hkl}^0}{d_{hkl}^0} = \frac{d_{hkl}}{d_{hkl}^0} - 1$$
  - Calculate stress: $\sigma = f_2(\varepsilon)$



- A complicated **inverse problem**:
  - Integration of mechanics, crystallography, materials science, diffraction physics

Engineering Diffraction: *Typical Experiment*

Typical engineering studies:

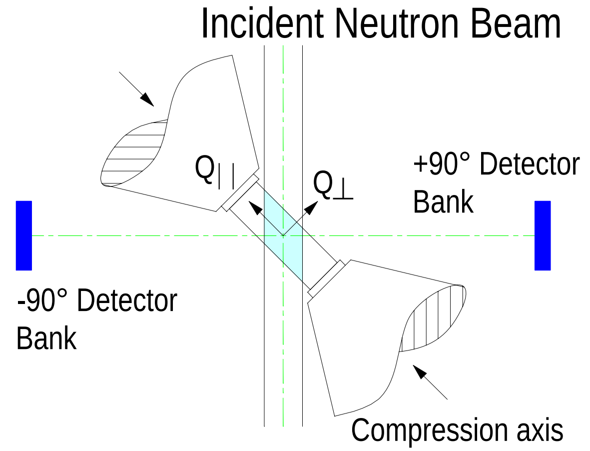
– Deformation studies
– Residual stress mapping
– Texture analysis
– Phase transformations

Eng. Diffractometers:

SMARTS (LANSCE)

ENGIN X (ISIS)

VULCAN (SNS)

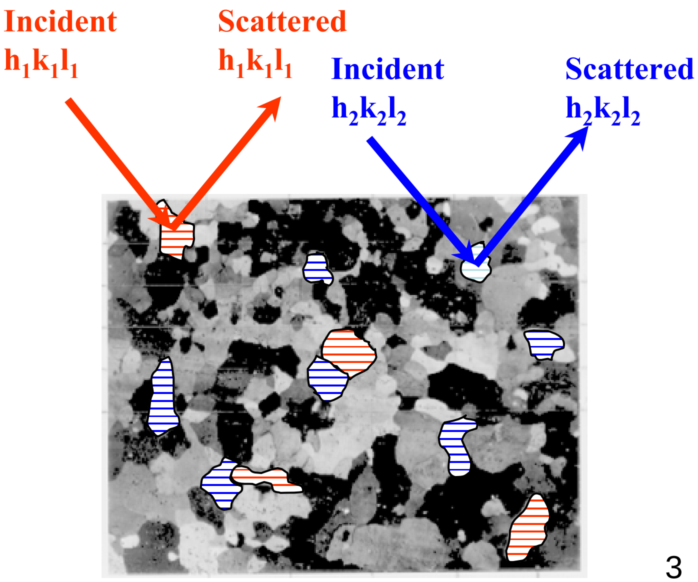


$$\varepsilon_{hkl}^{el} = \frac{d_{hkl} - d_{hkl}^{0}}{d_{hkl}^{0}} = \frac{d_{hkl}}{d_{hkl}^{0}} - 1$$

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

$$E_{hkl} = f_3(h,k,l)$$



Need for a sophisticated forward model of experiment

Engineering Diffraction: *Vision for DANSE*

- Objectives:
  - Enable new science (and enhance the value of EngND output)
  - Utilize beam time more efficiently
  - Help enlarge user community
- Approach:
  - Make it easy to use existing tools (e.g., *ABAQUS*)
  - Introduce new methods for existing tools (e.g., optimization); complex analysis
  - Develop new tools (e.g., experiment design and simulation)
  - Educate users (documentation, *"Expert System"*)
  - Conduct new science along the way (e.g., microstructure simulation)
- *DANSE* advantage: modularity, extensive libraries, new tools
- Impact:
  - Re-definition of diffraction stress analysis
  - Easy transfer to synchrotron *XRD*, *NDE analysis*, *damage prognosis*

Engineering Diffraction: *Plans for DANSE*

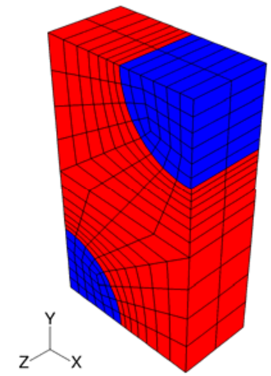
Proposed *Flagship* Applications

1. **Mechanics Modeling I**: finite element analysis (**FEA**):
   - *ABAQUS* integration
   - Model optimization via input from experiment
2. **Mechanics Modeling II**: self-consistent modeling (**SCM**):
   - *EPSC, etc.* integration
   - Model optimization via input from experiment
3. **Data Analysis**:
   - Diffraction data analysis (Rietveld and single-peak fitting)
   - Comparison to mechanics modeling
4. **Experiment Design and Simulation** (***"Expert System"***):
   - Instrument simulation (*McStas*)
   - Optimization of parameters
   - Microstructure simulation (*PolyViggen*)

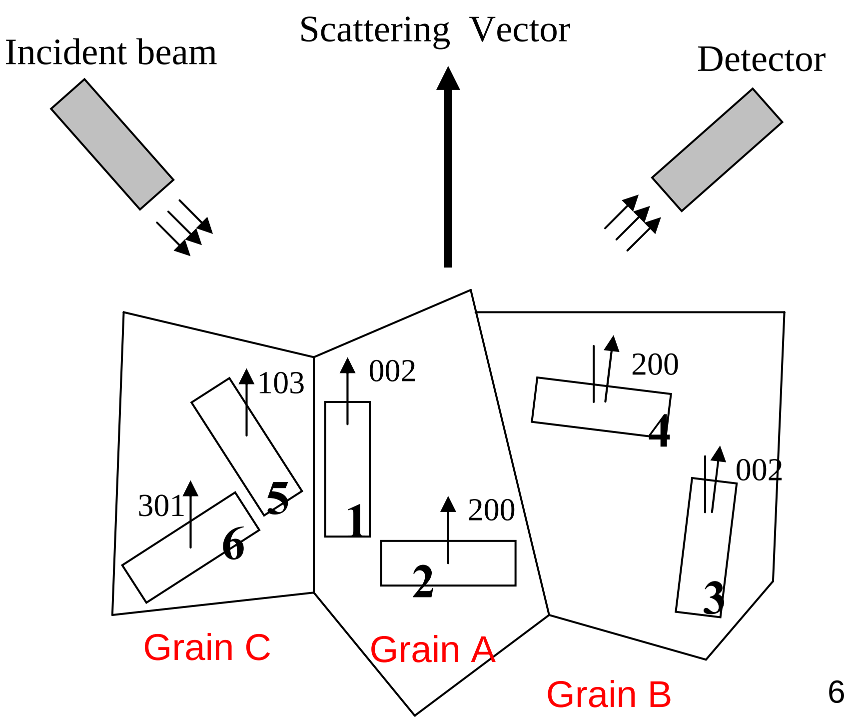
Efforts underway in all of these tasks

Mechanics Modeling

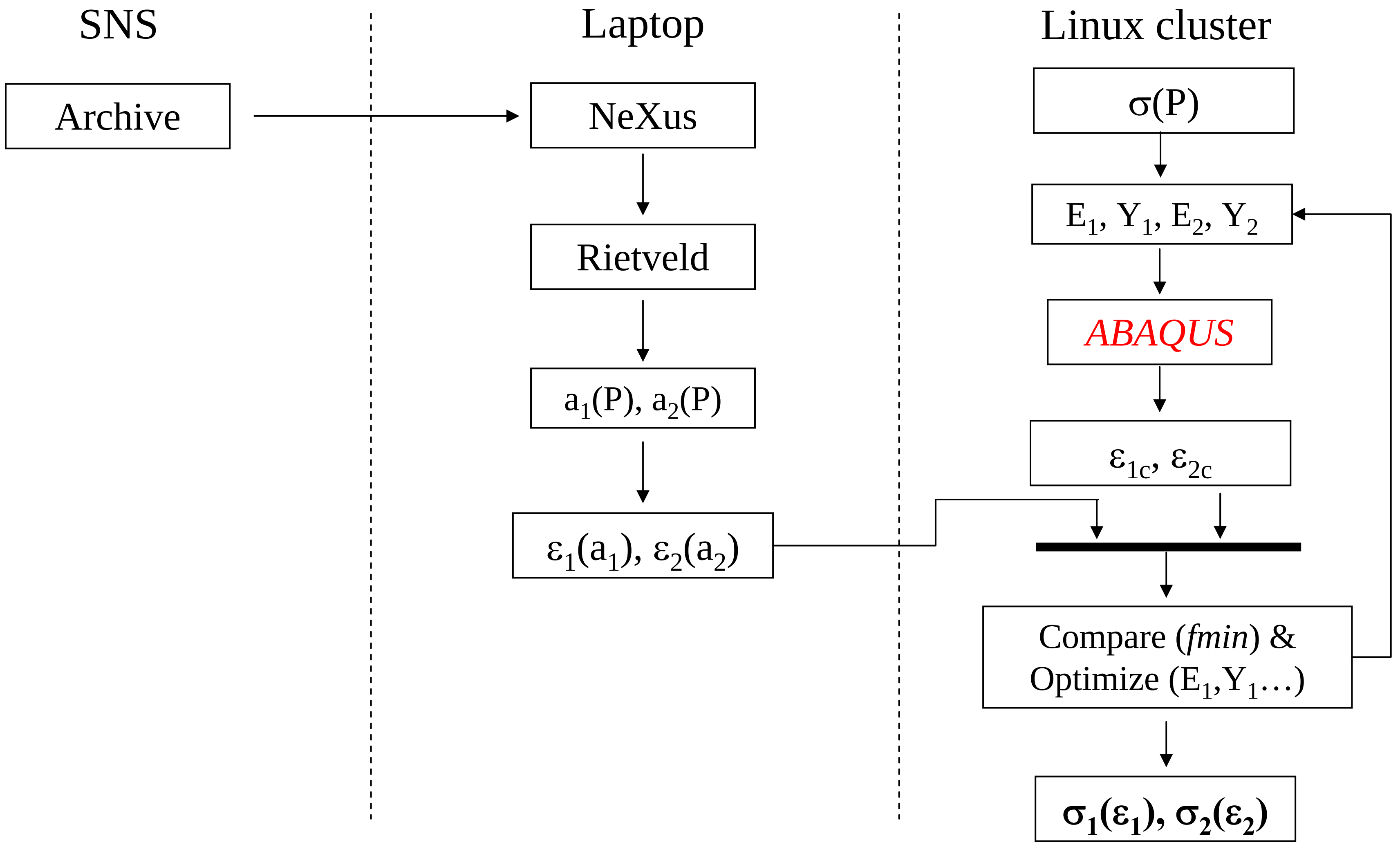
- Finite element analysis (FEA)
  - *ABAQUS*
  - Optimization of material parameters



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

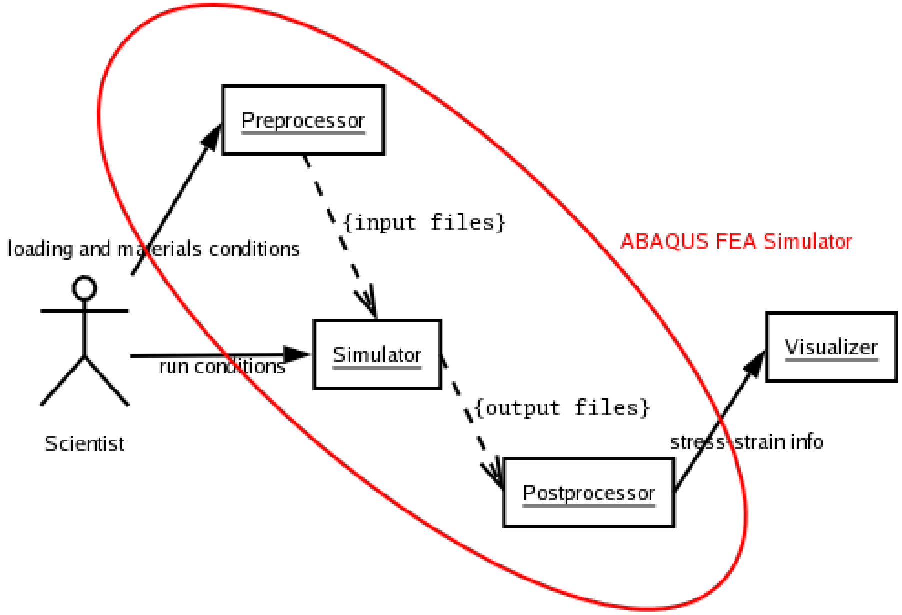


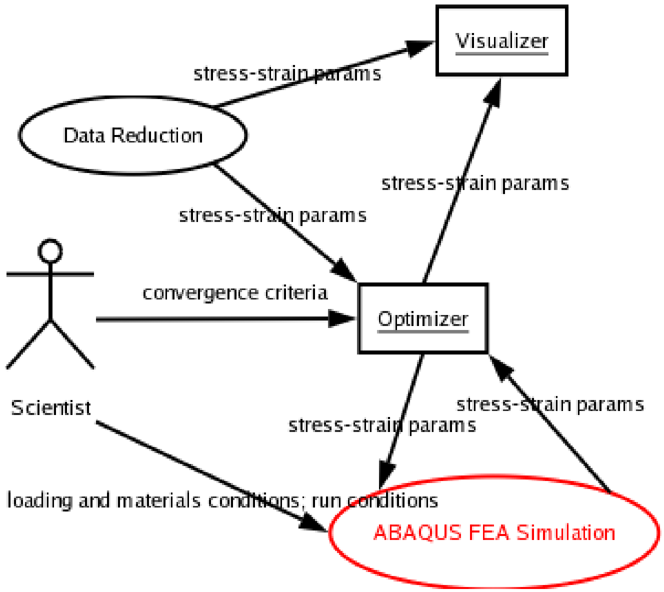
Mechanics Modeling: *FEA* (Finite Element Analysis)



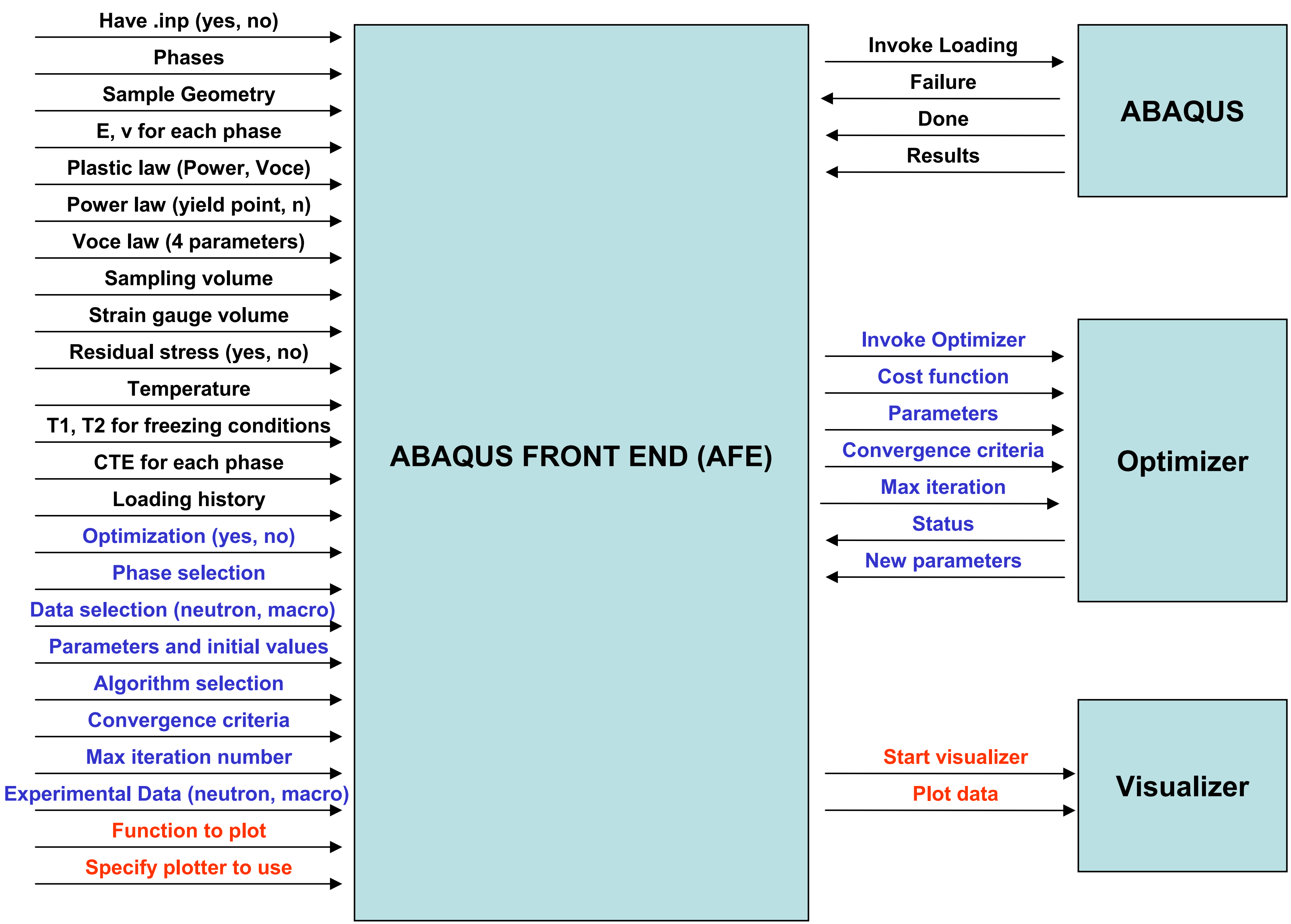
ABAQUS: **High Level Use Case Diagram**

Planned release: Summer 2007

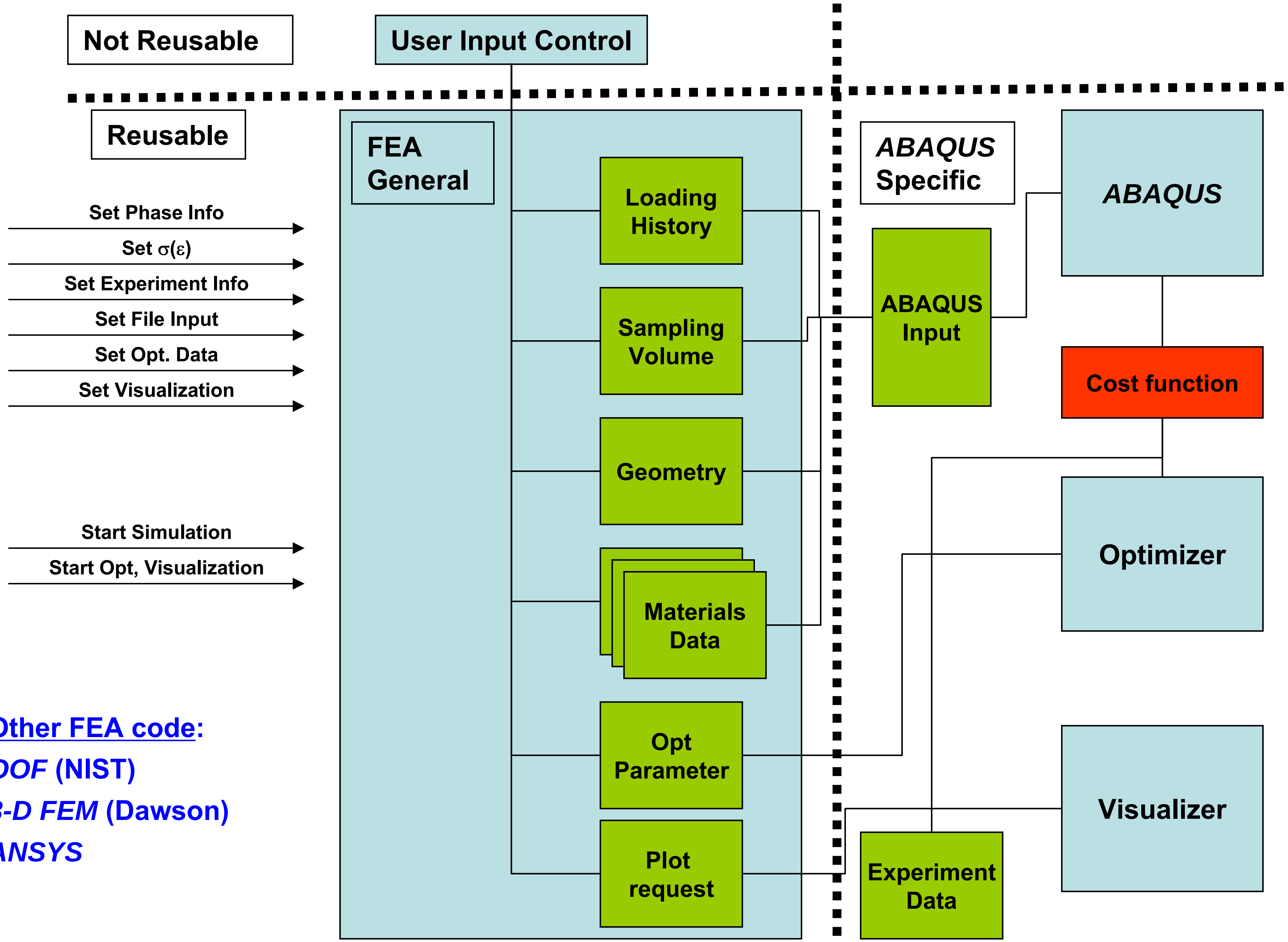




ABAQUS: **System Boundary**



ABAQUS: Stimulus and Abstract Classes



Other FEA code:

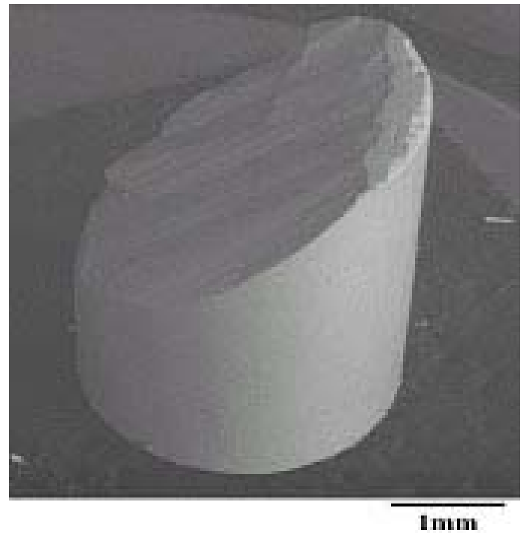
***OOF* (NIST)**

***3-D FEM* (Dawson)**

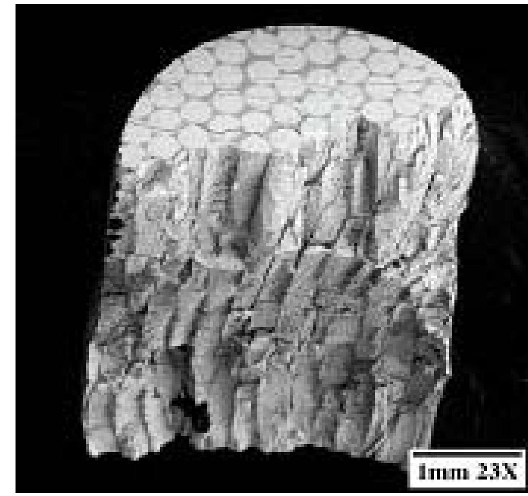
ANSYS

ABAQUS Example: *BMG-W fiber composite*

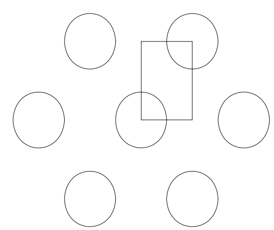
- Residual stresses
- Compression loading at SMARTS
- Experiments on 20% to 80% volume fraction of W
- Unit cell finite element model
- Rietveld (*GSAS*) output for average elastic strain in W in the longitudinal direction



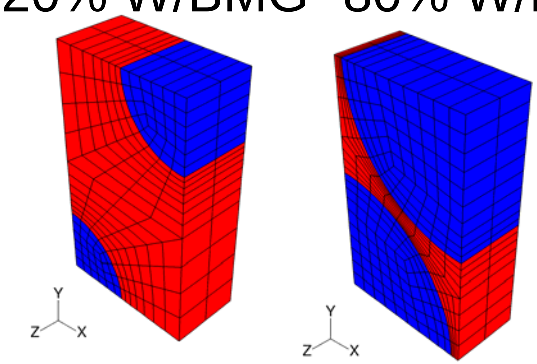
BMG



W-BMG composite



20% W/BMG 80% W/BMG

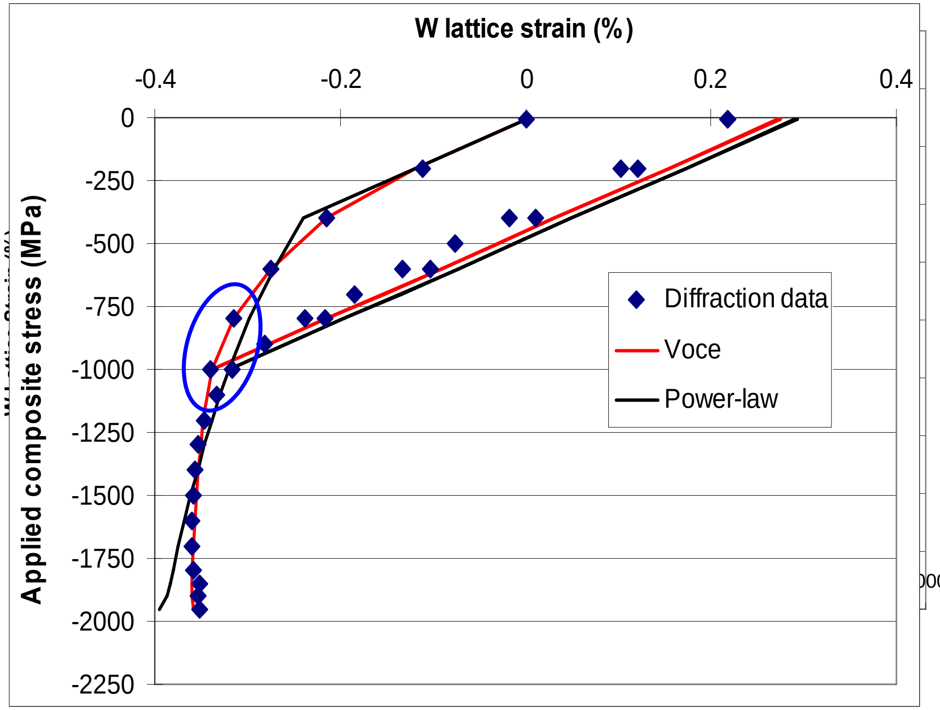


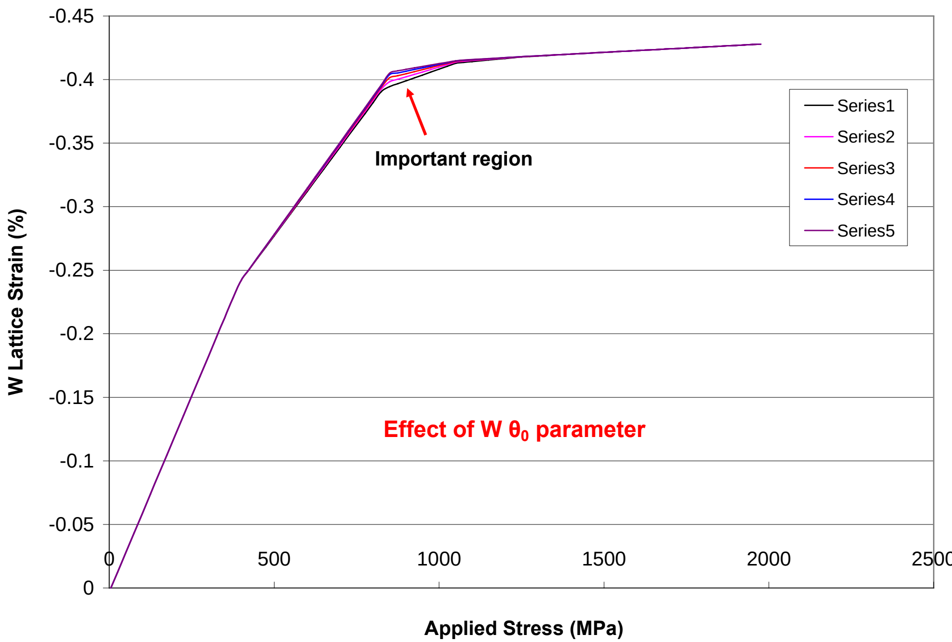
Reference: B. Clausen et al., Scripta Mater. 49 (2003) p. 123

ABAQUS + Neural Network Analysis

New use of current tools

Sensitivity Studies





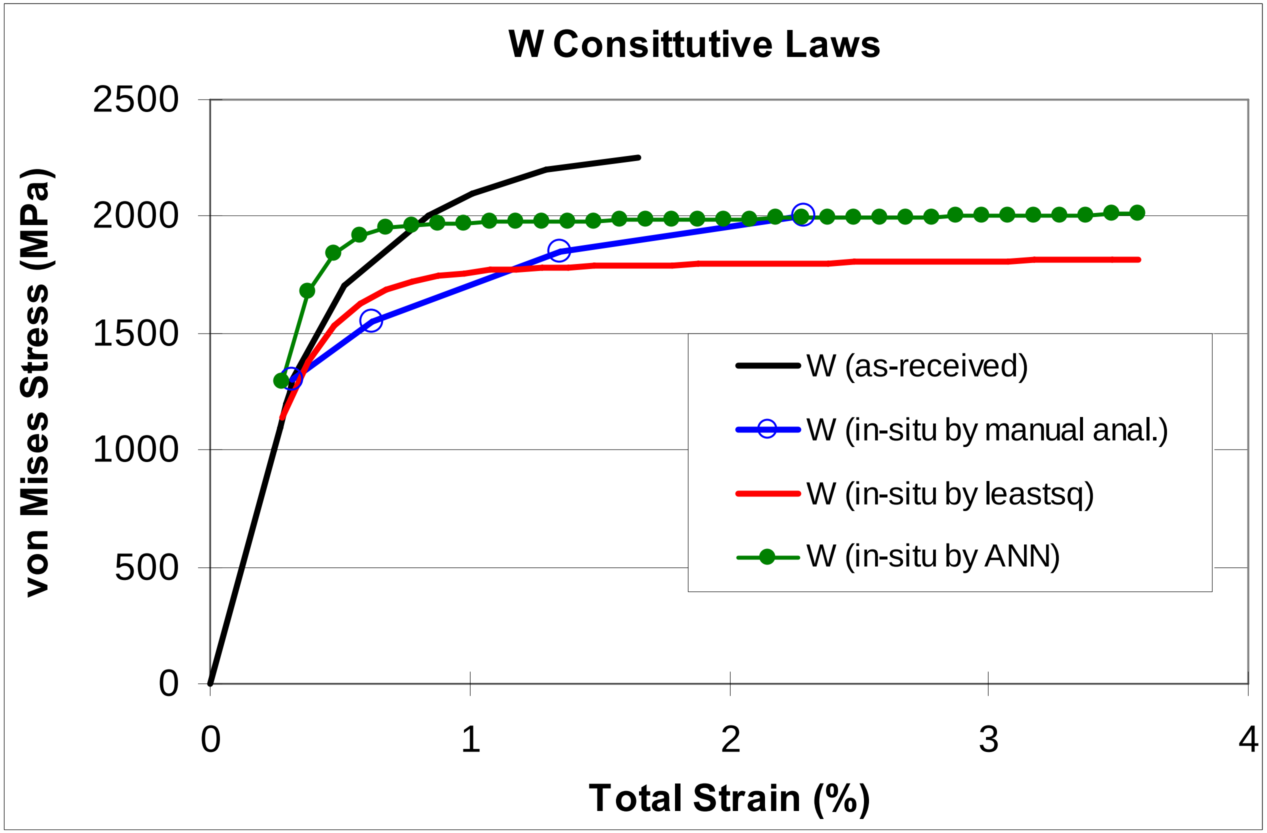
- **Strong influence by parameters: $(\sigma_0)_{BMG}$, $(\sigma_0)_W$, $(\sigma_1)_W$ and $(\theta_0)_W$**
- **Weak/no influence by parameters: n_{BMG}, $(\theta_1)_W$ and ΔT**
- ***Rigorous experiment planning to optimize data collection***

L. Li *et al.*

ABAQUS + 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



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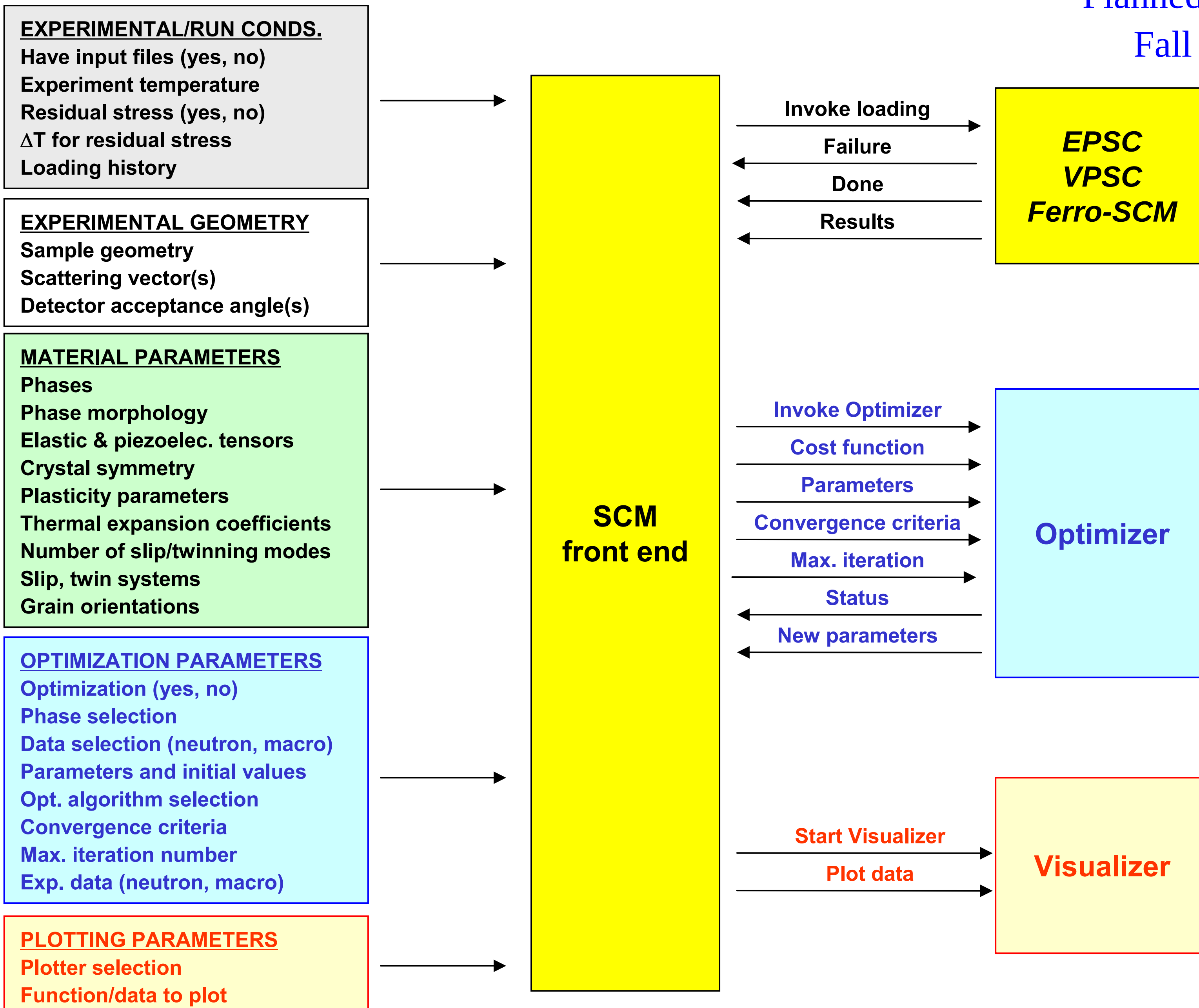
Self-Consistent Modeling: System Boundary

Planned release:
Fall 2007

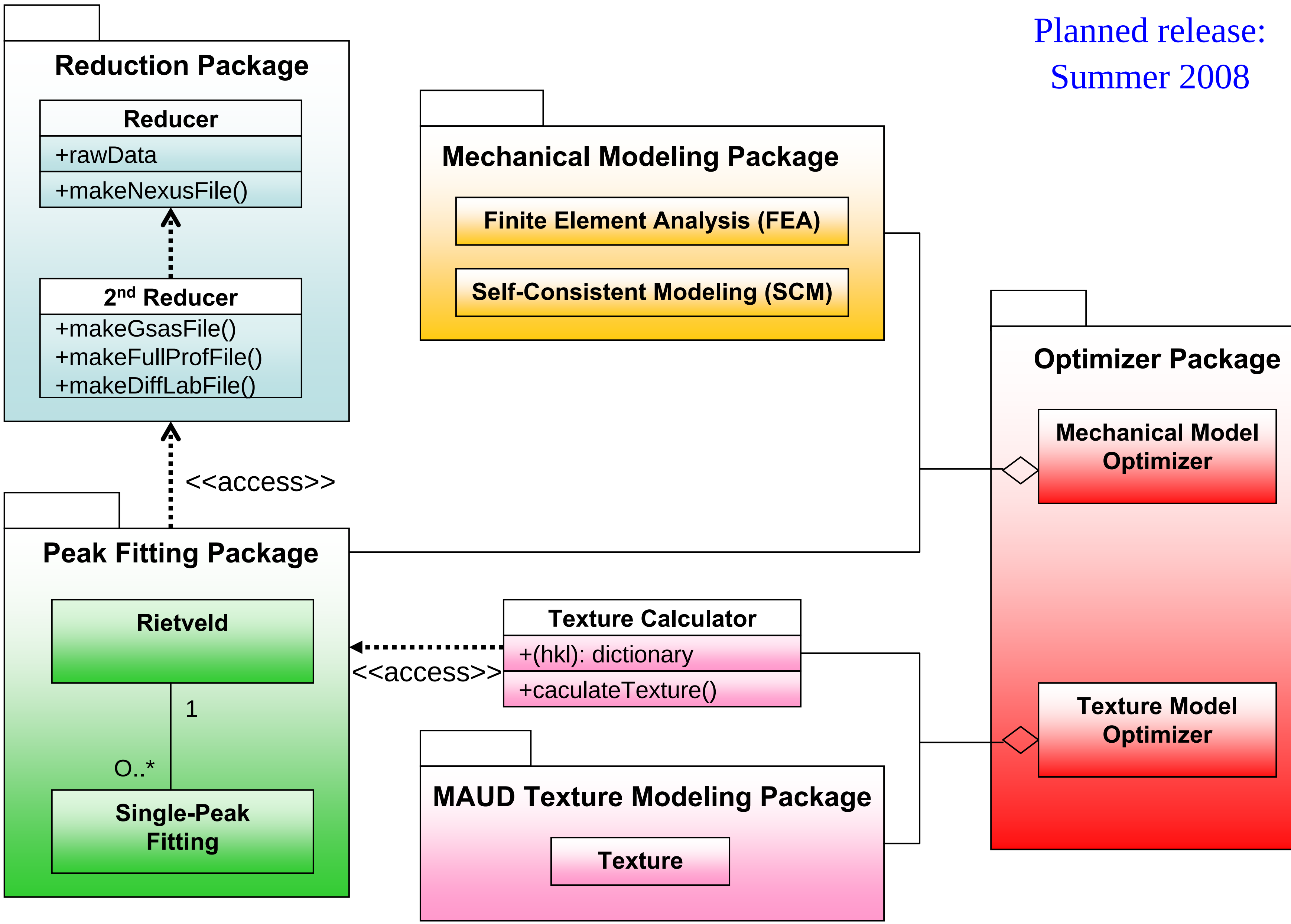


Data Analysis

- 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

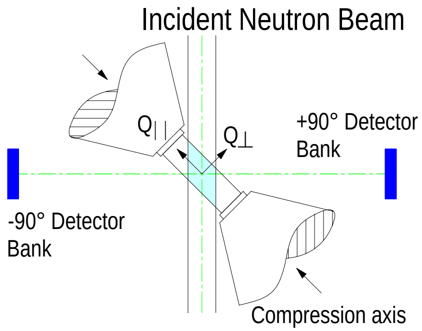
Data Analysis: **High Level Use Case Diagram**

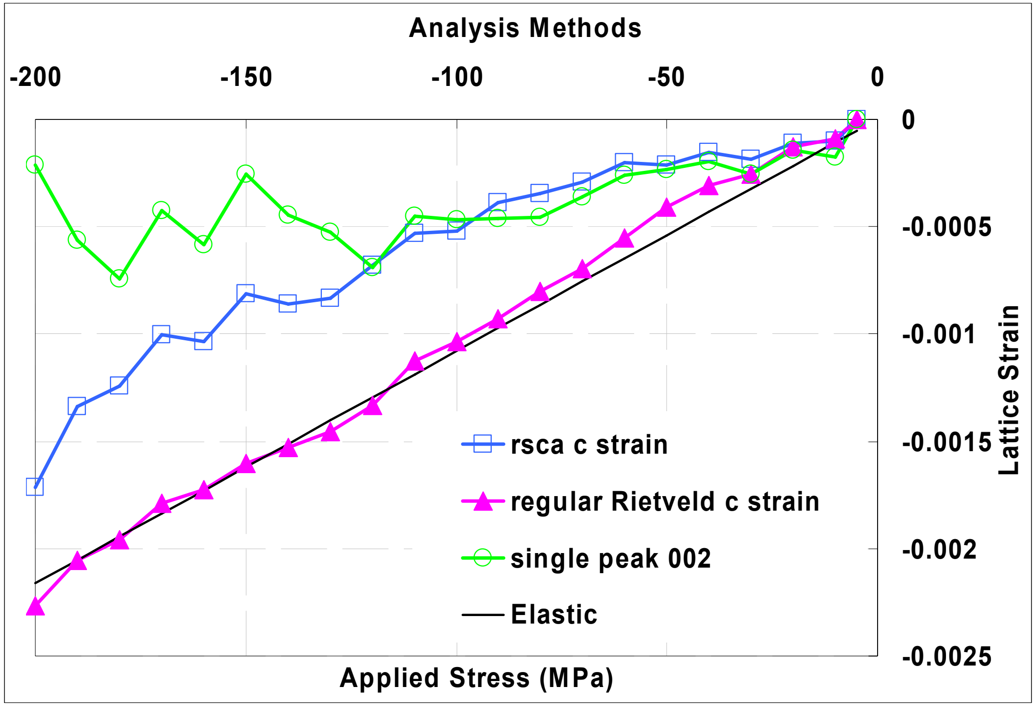
Planned release:
Summer 2008



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

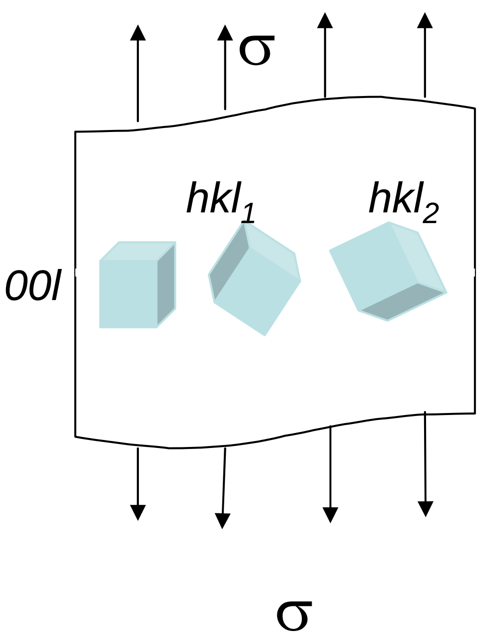
Different data analysis approaches:

- 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

Diffraction Strain Analysis: *Cubic Materials*

$$\varepsilon_{hkl} = \frac{d_{hkl} - d^0_{hkl}}{d^0_{hkl}} \qquad d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad \Rightarrow \quad \varepsilon_{hkl} = \frac{a - a^0}{a^0}$$

$$\frac{1}{E_{hkl}} = \underbrace{S_{11}}_{Isotropic} - \underbrace{2(S_{11} - S_{12} - S_{44}/2)A_{hkl}}_{Anisotropic} \qquad A_{hkl} = \frac{(h^2k^2 + k^2l^2 + l^2h^2)}{(h^2 + k^2 + l^2)^2}$$



Grains experience different strains based on their orientation and elastic anisotropy

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

Correction needed in strain analysis via Rietveld

Reuss (equal stress) assumption:

$$\varepsilon_{hkl} = \frac{\sigma}{E_{hkl}}$$

Diffraction Strain Analysis: *Hexagonal Materials*

New science

New use of current tools

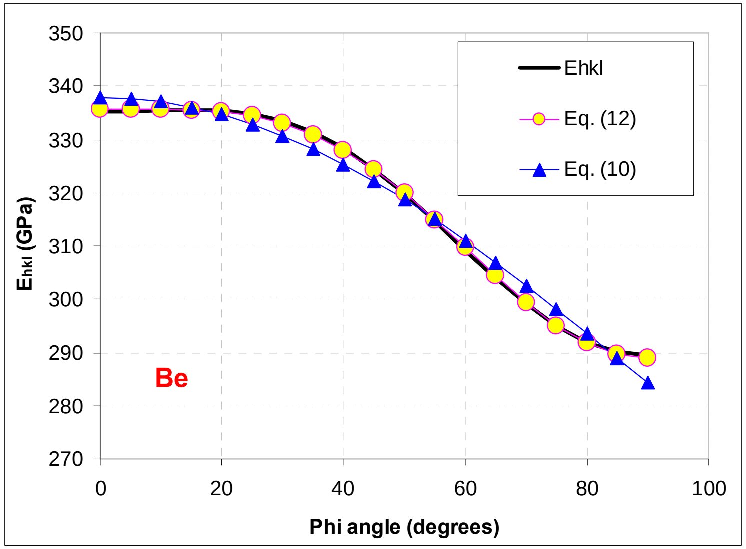
$$d_{hkl}^2 = \frac{1}{\frac{4}{3}\left(\frac{h^2+hk+k^2}{a^2}\right)+\frac{l^2}{c^2}}$$

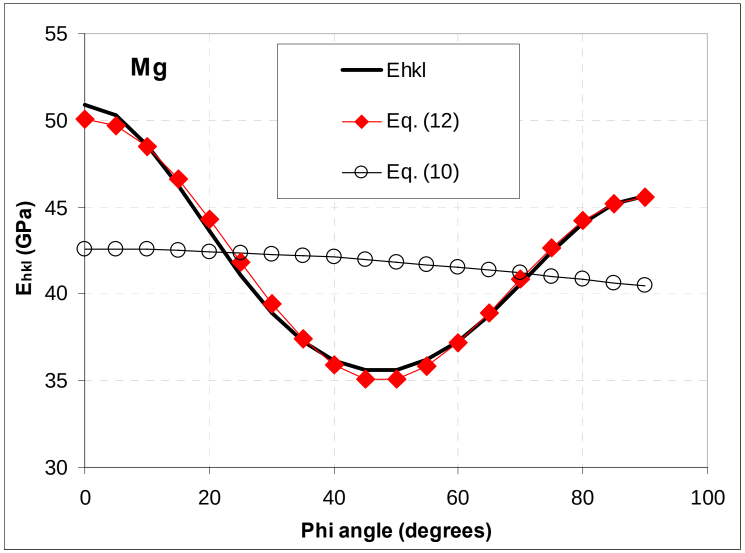
$$\frac{1}{E_{hkl}} = (1-l_3^2)^2 S_{11} + l_3^4 S_{33} + l_3^2(1-l_3^2)(2S_{13}+S_{44})$$

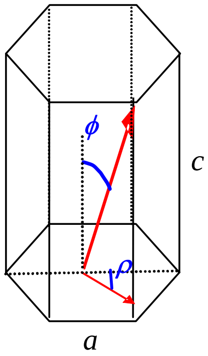
$$\varepsilon_{hkl} = \varepsilon_{isotropic} + \gamma \cos\phi \qquad (10)$$

- Three refineable parameters (γ_i)
- E_{hkl} equation exact
- Good fits for Be and Mg

$$\varepsilon_{hkl} = \varepsilon_{isotropic} - \gamma_1(1-l_3^2)^2 - \gamma_2 l_3^4 - \gamma_3 l_3^2(1-l_3^2) \qquad (12)$$







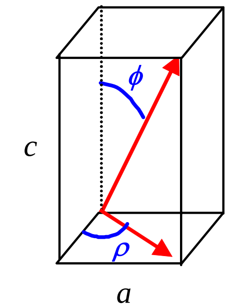
Diffraction Strain Analysis: *Tetragonal Materials*

New science

New use of current tools

$$d_{hkl}^{2} = \frac{1}{\left(\frac{h^2+k^2}{a^2}\right) + \frac{l^2}{c^2}}$$

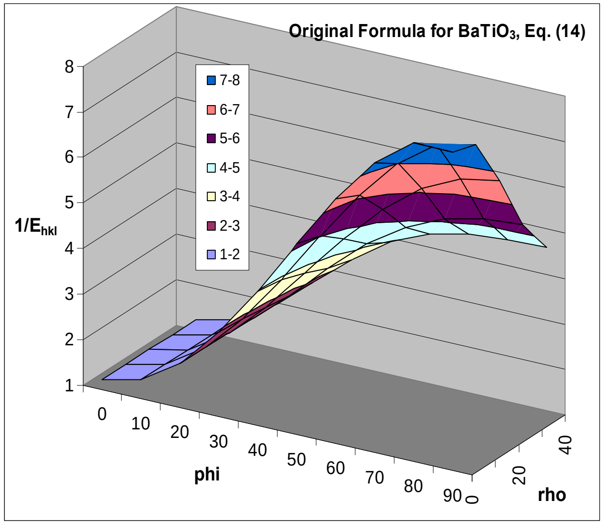
$$l_1 = \sin\phi.\sin\rho; \qquad l_2 = \sin\phi.\cos\rho; \qquad l_3 = \cos\phi$$

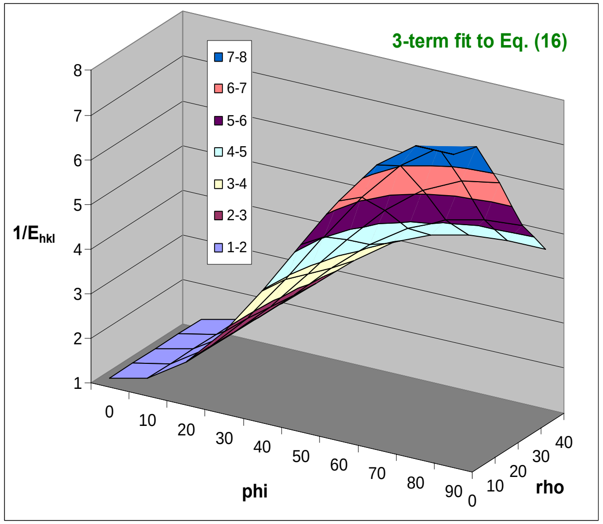


$$\frac{1}{E_{hkl}} = (l_1^4 + l_2^4)S_{11} + l_3^4 S_{33} + l_1^2 l_2^2 (2S_{12} + S_{66}) + l_3^2(1 - l_3^2)(2S_{13} + S_{44}) \quad (14)$$

$$\varepsilon_{hkl} = \varepsilon_{isotropic} + \gamma_1(l_1^4 + l_2^4) + \gamma_2 l_3^4 + \gamma_3 l_1^2 l_2^2 + \gamma_4 l_3^2(1 - l_3^2) \quad (16)$$

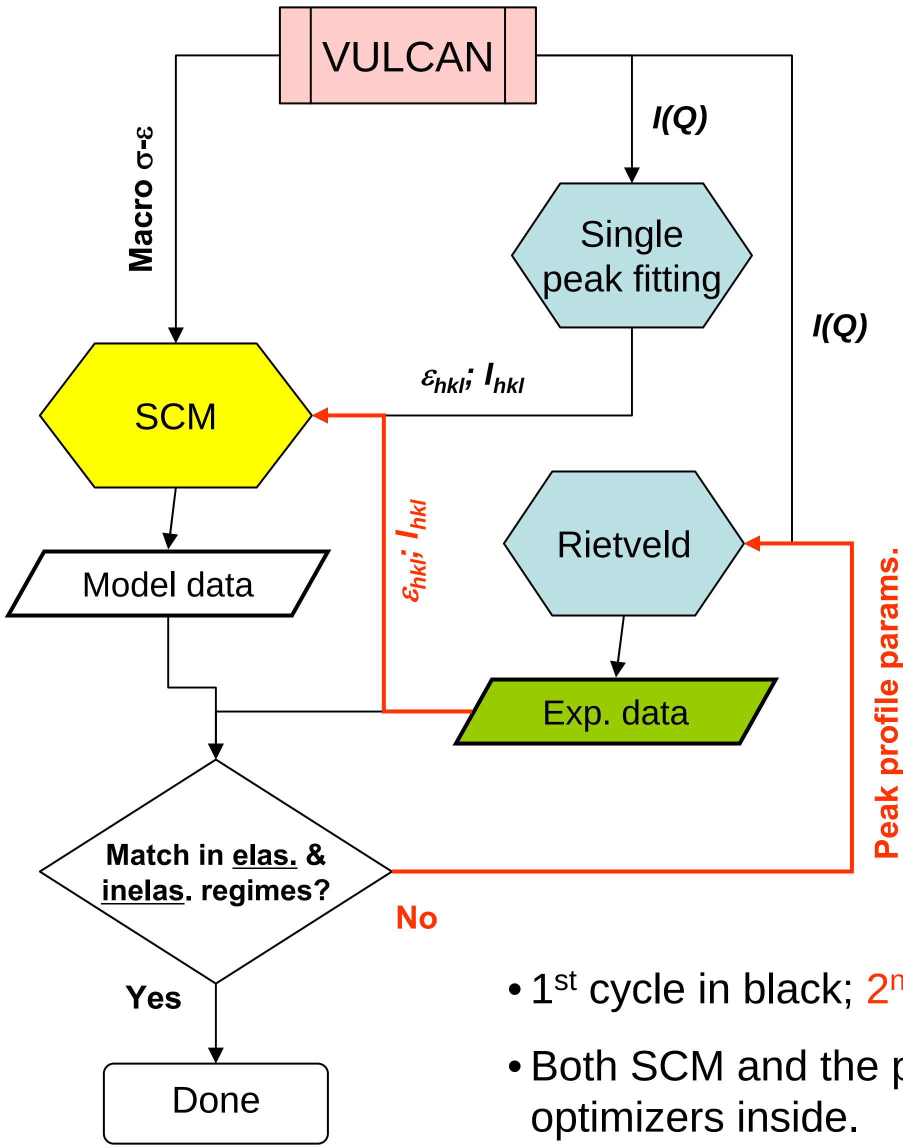
Very good fit for tetragonal E_{hkl} *with 3 parameters*





G. Tutuncu *et al.*

Integration of Crystallographic and Mechanics Models



- Integration of peak fitting with self-consistent model (SCM)
- Iterative refinement of SCM & Rietveld
- Rigorous determination of constitutive law

New science

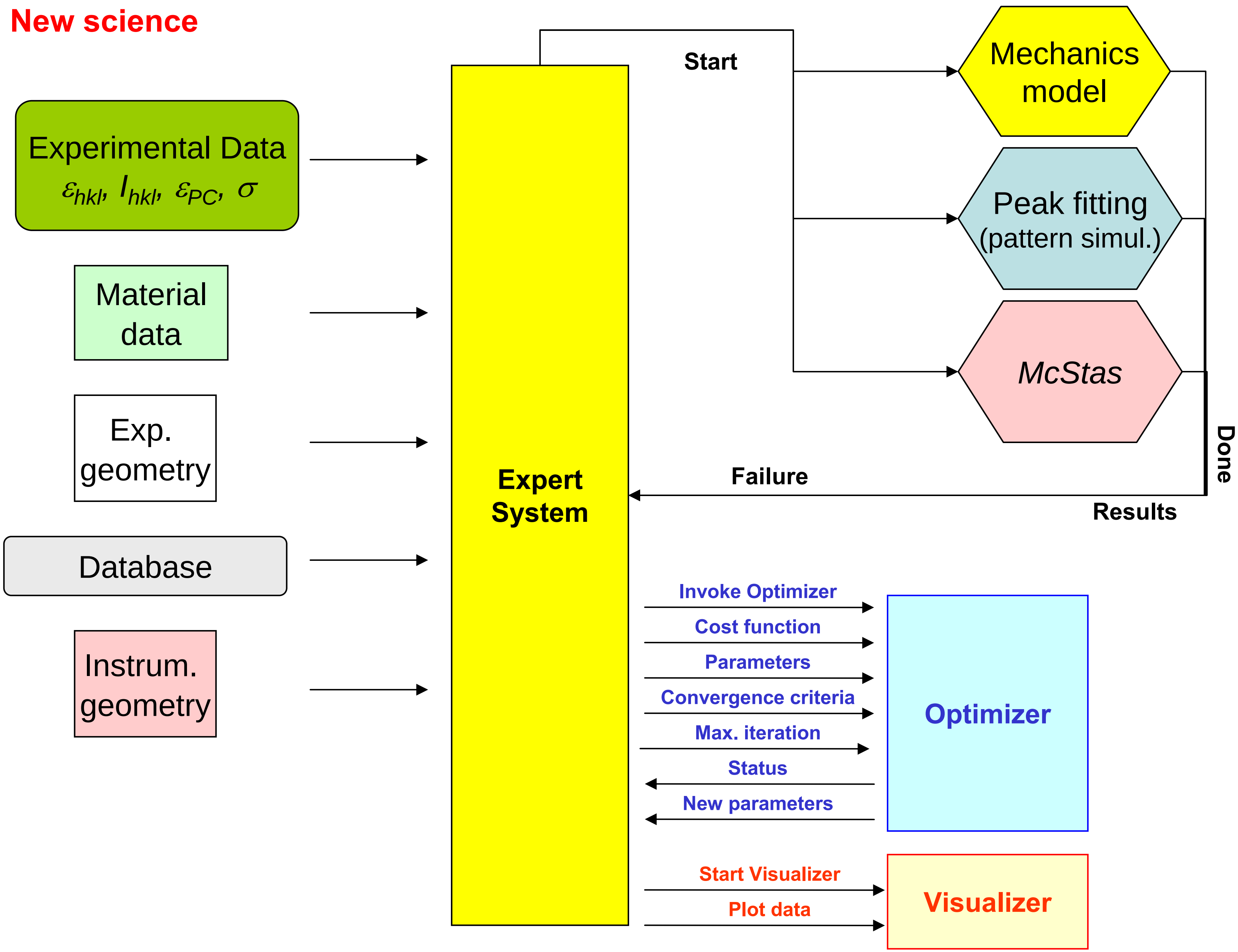
New use of current tools

- 1st cycle in black; 2nd cycle in red.
- Both SCM and the peak fitting routines have optimizers inside.

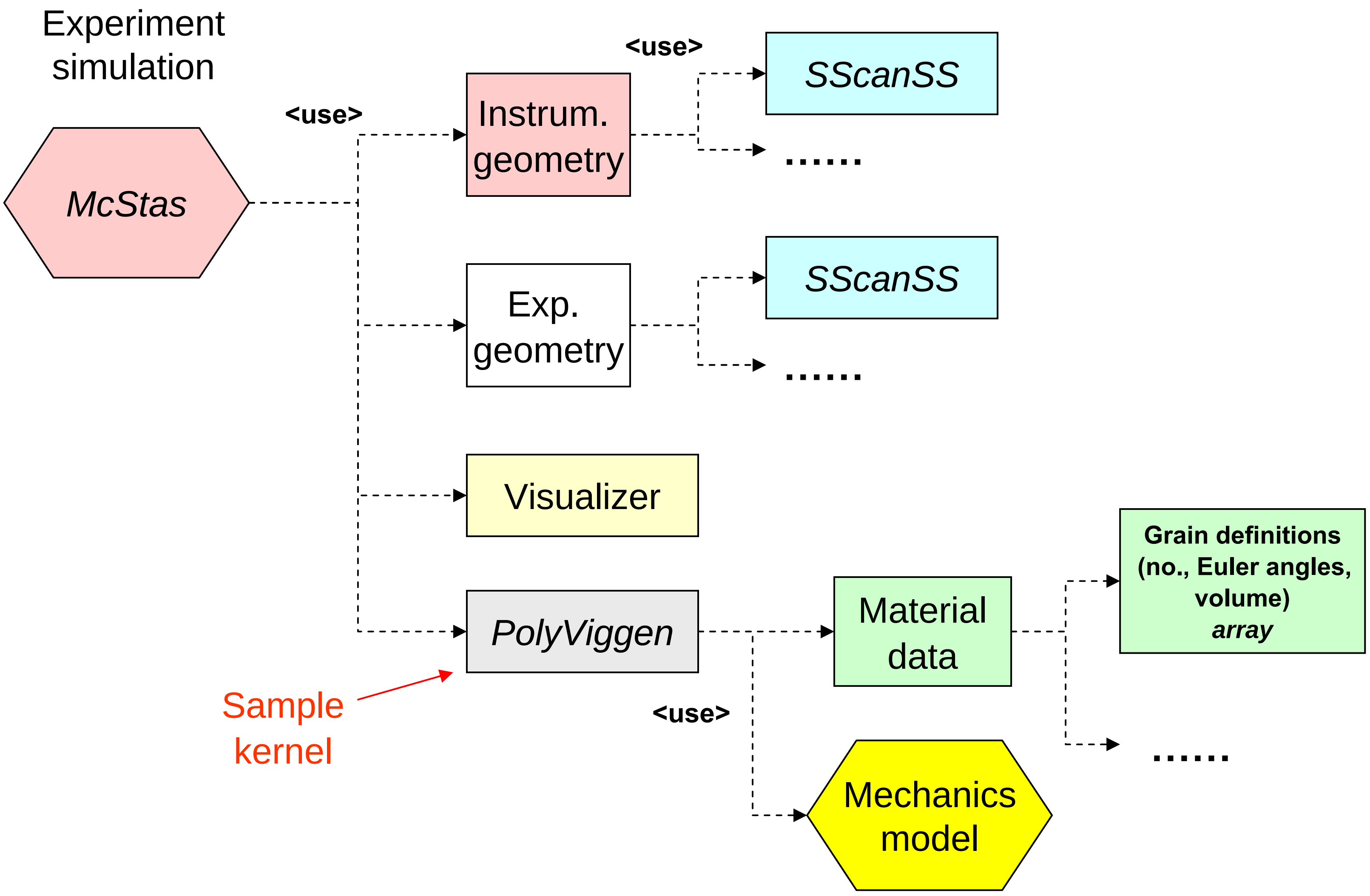
Experiment Design and Simulation

- 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**

“Expert System”: **System Boundary**



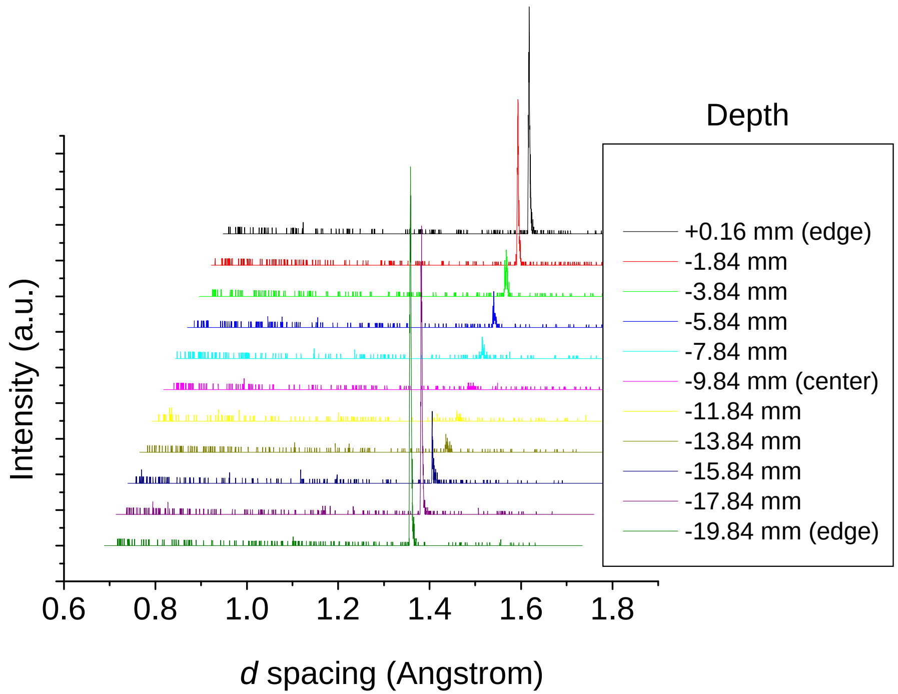
“Expert System”: **Stimulus and Abstract Classes**

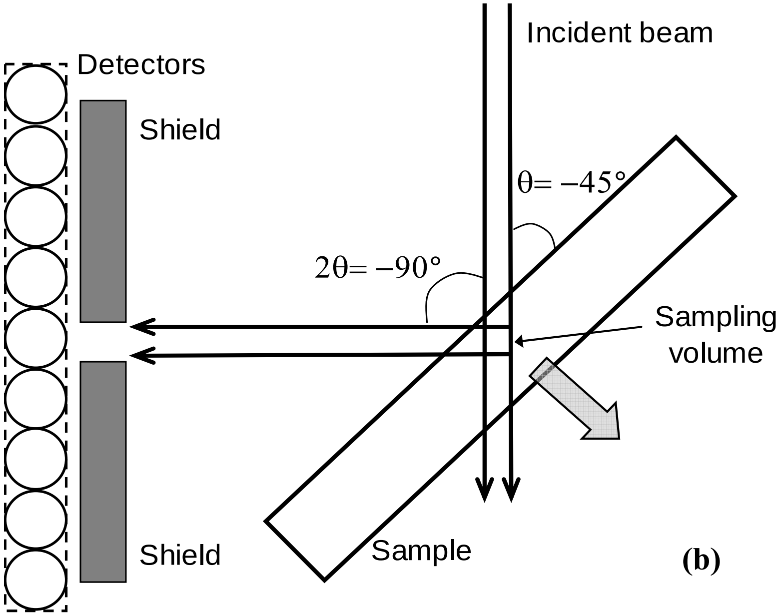


Microstructure Simulation

New science

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





Critical question: *Transition between a single crystal and polycrystal?*

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

Engineering Diffraction: *Team*

- E. Üstündag[‡], S.Y. Lee, S.M. Motahari, G. Tutuncu (ISU) + **undergrads** (J. Barthel, J. Jones)
- X.L. Wang[‡] (SNS) - *VULCAN*
- I.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*

New skills for young scientists

Internal training

Community involvement

‡ Member of EngND Executive Committee