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The Inadequacy of Uncertainty Estimation in Residual Stress Measurements

And some ideas on what to do about it

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NNSA
National Nuclear Security Administration

Ignorance is not probabilistic.

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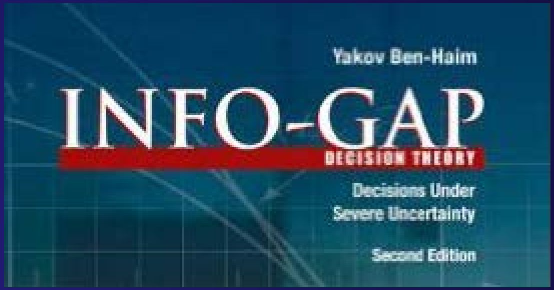

So we generally end up with a lower bound estimate of uncertainty

Not conservative

Outline

- **Motivation**
- **Conventional uncertainty estimation**
- **Two examples of *demonstrably* underestimated uncertainties, with improvements proposed**
  - Incremental slitting: improving the *analytical* estimation of uncertainty
  - Neutron diffraction: improving uncertainty estimation using additional *data*
- **Thoughts**

Motivation

- **In the context of structural integrity, life prediction, and structural health monitoring, for example, …**
- **Uncertainties *on the important quantities* …**
  - Lifetime, crack growth rate, stress corrosion cracking rate, ….

Are vital for protecting human life and assets while minimizing cost/weight/inspections, etc.

- **For the purposes of this talk, we assume that uncertainties on residual stress measurements and/or predictions are a necessary part of that**

Standard uncertainty

- **The overwhelming majority of uncertainty estimates come from the standard error propagation equation**

Let *f(x,y)* be a function of two variables, and assume that the uncertainties on *x* and *y* are known and "small". Then:

$$\sigma_f^2 = \left(\frac{df}{dx}\right)^2 \sigma_x^2 + \left(\frac{df}{dy}\right)^2 \sigma_y^2 + 2\left(\frac{df}{dx}\right)\left(\frac{df}{dy}\right)\rho\,\sigma_x\sigma_y$$

(Note that I have included the cross-terms, which cannot always be ignored)

- **Where we propagate the uncertainty in the main measured quantity (e.g., strain, diffraction peak location, …) and usually nothing else**

<u>This approach is often inadequate for two reasons:</u>

1. We do not propagate all of the uncertainties
2. This approach is inadequate in itself

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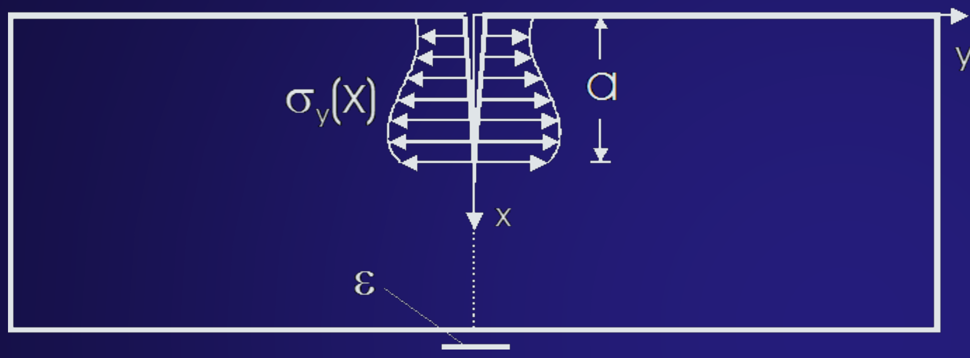
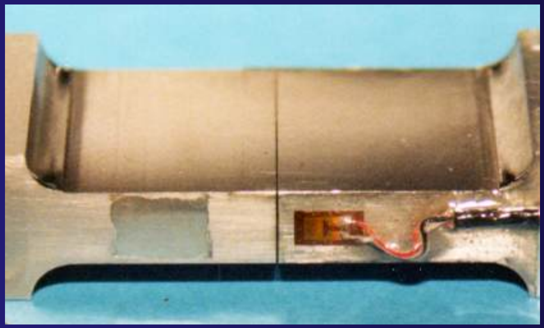
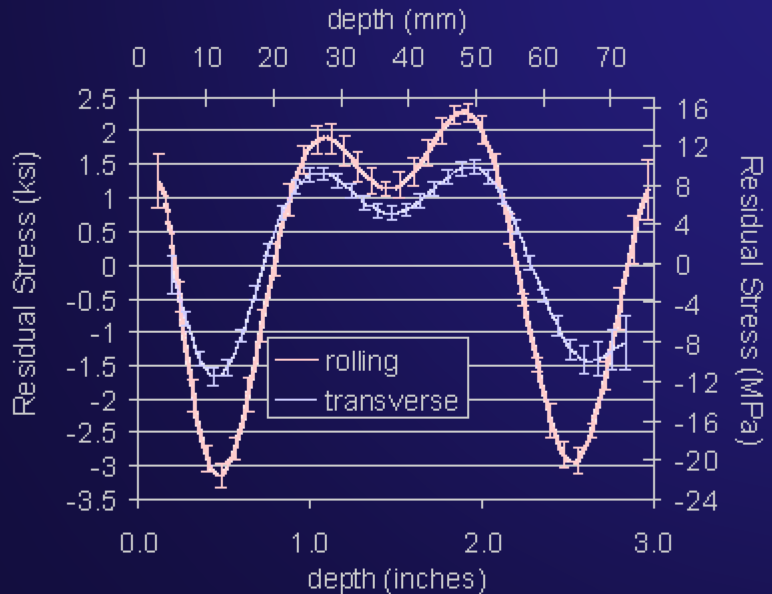
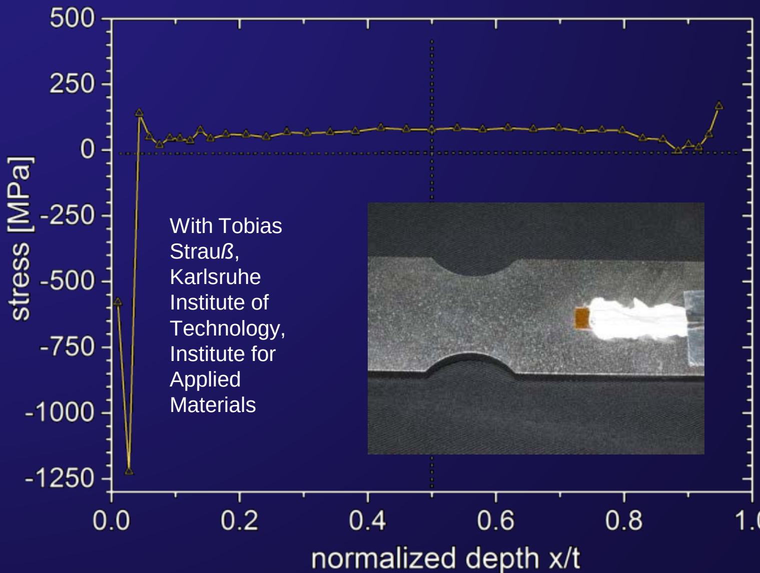
The slitting method is a powerful tool for measuring a depth profile of residual stresses









Uncertainty propagation through least squares fit inverse

$$\sigma_y(x_i) = \sigma_i = \sum_{j=1}^{n} A_j P_j(x_i) = [P]\{A\}$$

$$\{A\} = \left[\left([C]^T[C]\right)^{-1}[C]^T\right]\{\varepsilon\} = [B]\{\varepsilon\}$$

$$s_i^2 = u_{A_1}^2\left(\frac{\partial\sigma_i}{\partial A_1}\right)^2 + u_{A_2}^2\left(\frac{\partial\sigma_i}{\partial A_2}\right)^2 + \ldots + 2u_{A_1A_2}^2\left(\frac{\partial\sigma_i}{\partial A_1}\right)\left(\frac{\partial\sigma_i}{\partial A_2}\right) + \ldots$$

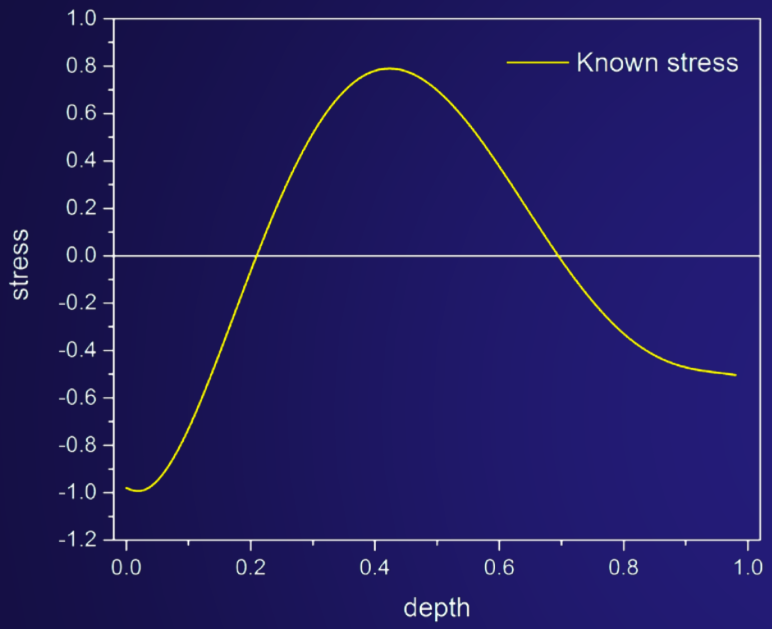
$$\frac{\partial\sigma_i}{\partial A_j} = P_j(x_i) \qquad \{s_i^2\} = \mathrm{diag}\left([P][V][P]^T\right)$$

$$V_{kl} = u_{A_kA_l}^2 = \sum_{i=1}^{m}\left[u_{\varepsilon,i}^2\frac{\partial A_k}{\partial\varepsilon_i}\frac{\partial A_l}{\partial\varepsilon_i}\right] \qquad \frac{\partial A_k}{\partial\varepsilon_i} = B_{ki} \qquad [V] = [B]\left[\mathrm{DIAG}\{u_\varepsilon^2\}\right][B]^T$$

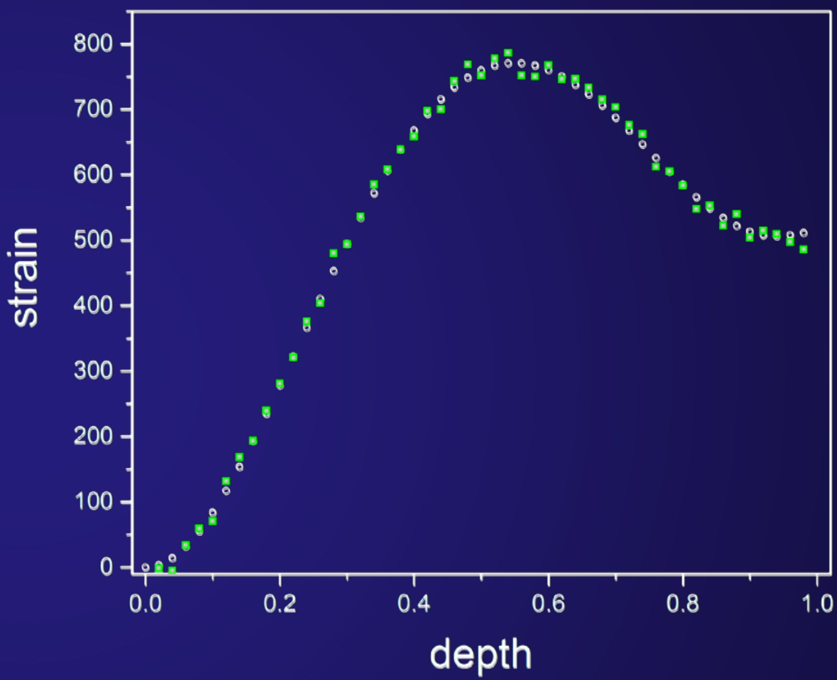
$$\{s_i^2\} = \mathrm{diag}\left([P]\left[\left([C]^T[C]\right)^{-1}[C]^T\right]\left[\mathrm{DIAG}\{u_\varepsilon^2\}\right]\left[\left([C]^T[C]\right)^{-1}[C]^T\right][P]^T\right)$$

Let's test it analytically

- **Pick a test stress profile**

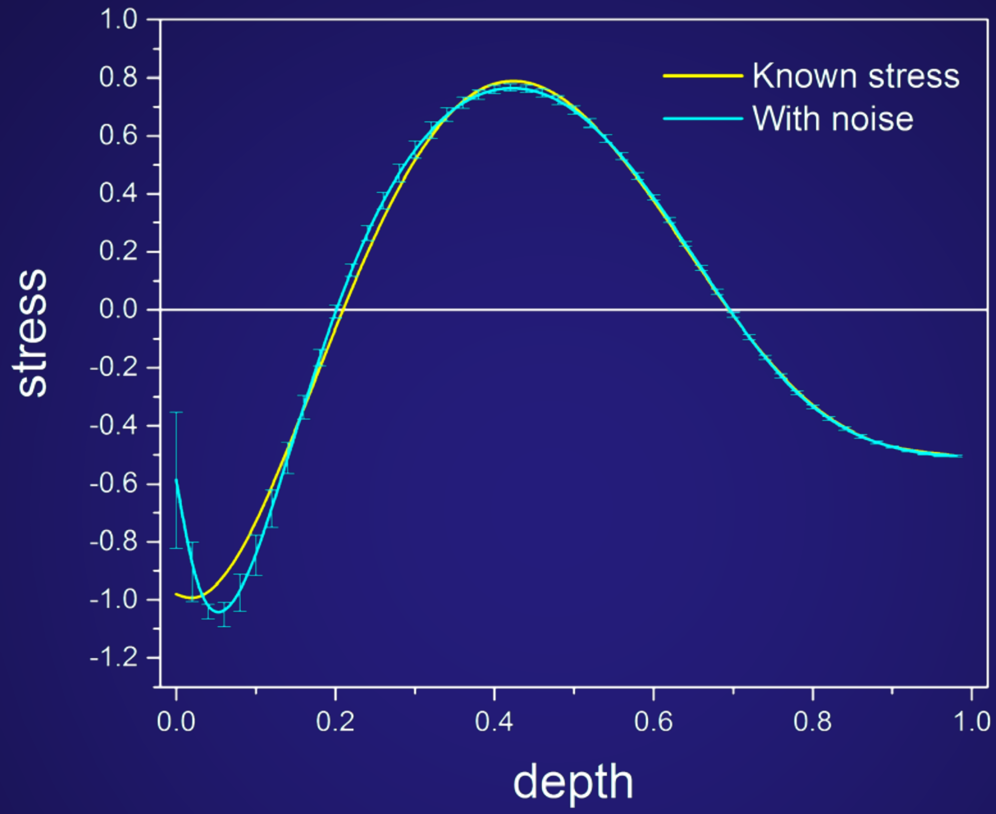


- **Use FEM to generate strain "data"**



- **Add some Gaussian random noise to the data**
- **Calculate stress and estimate errors**

Uncertainty analysis seems to work well



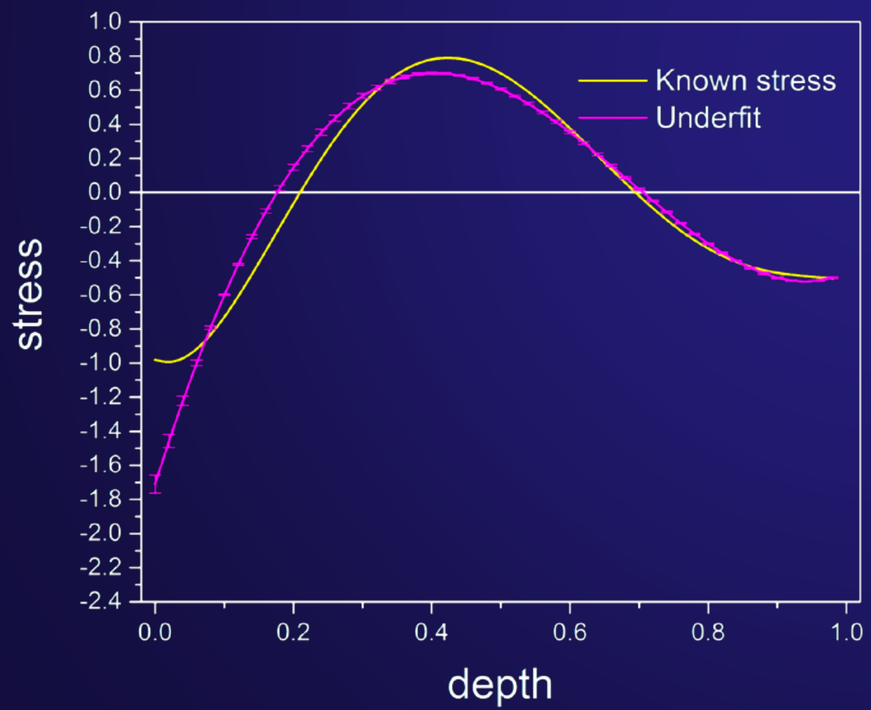
- **These are one standard deviation error bars (for the whole talk)**
  - So they should only encompass about 68% of the distribution

The only way to test a hypothesis is to look for all the information that disagrees with it

Sir Karl R. Popper
Austrian-British philosopher of science
Proponent of falsificationism

More general case?

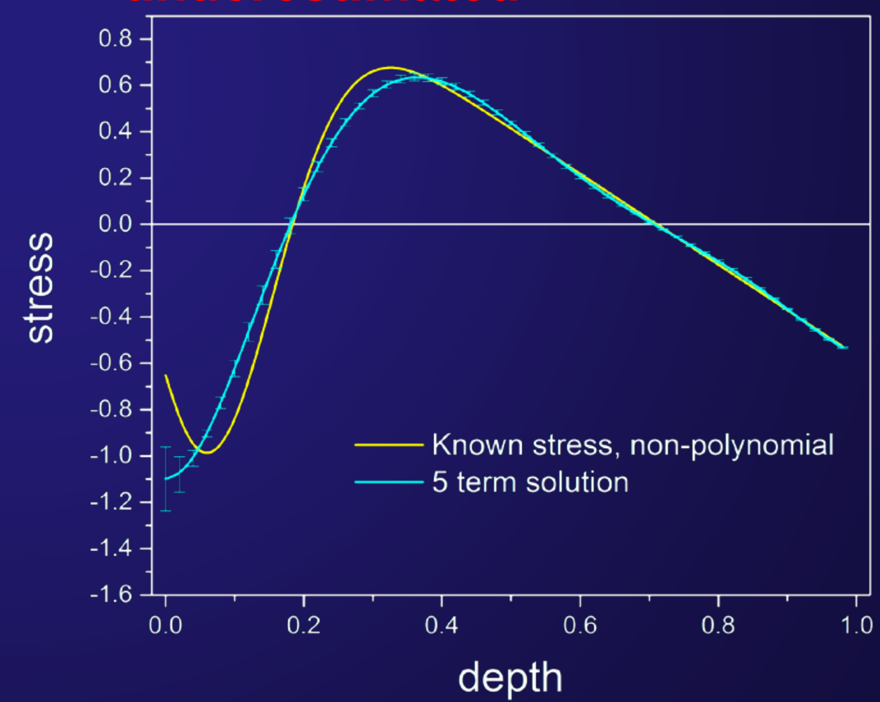
- **The test case was a 4th order polynomial**
- **What if I solve the inverse problem with only 3rd order?**
  - After all, you do not know what the “right” order is



- **Or with a profile that is not polynomial at all**

$$\sigma(x) = 2.28735\left(0.609825 - 0.857365x - e^{-\left(\frac{x-0.05}{0.15}\right)^2}\right)$$

- **Uncertainty is grossly underestimated**



What to do?

- **We usually estimate uncertainty based on uncertainty in the measured quantity:**

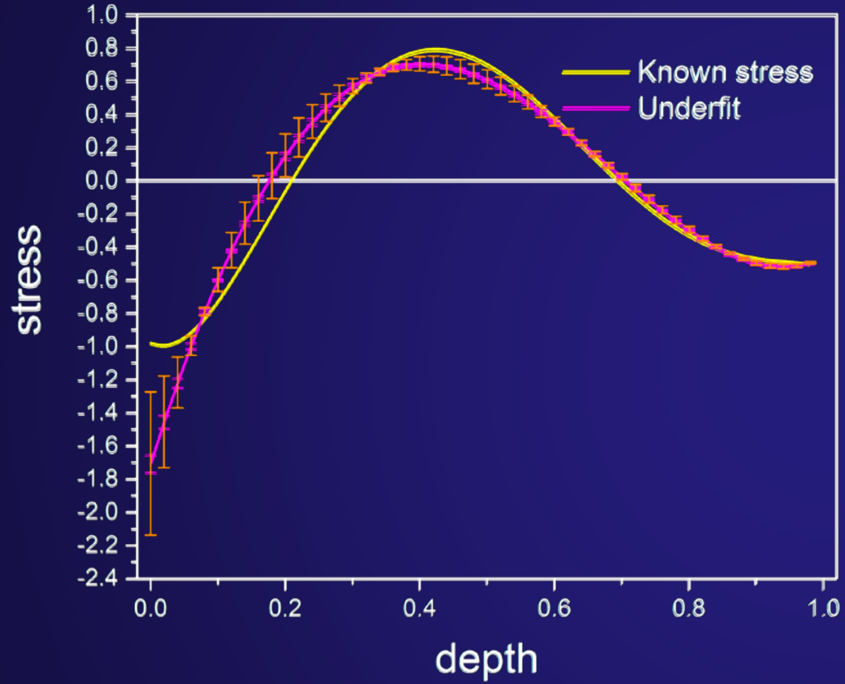
$$\partial \varepsilon_i$$

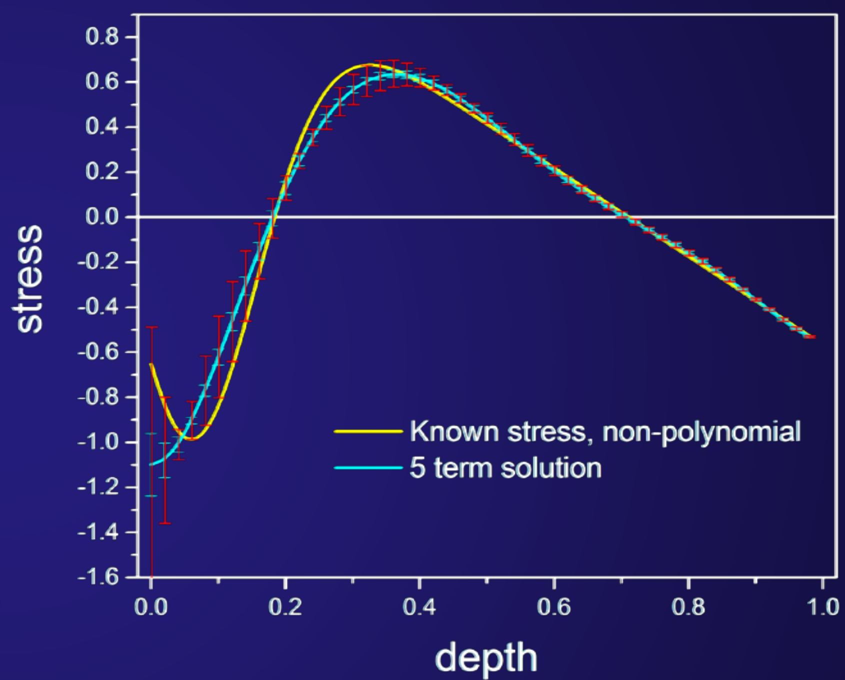
- **But really our choice of the "model" to represent the stress profile is equally uncertain**

$$\sigma_y(x_i) = \sigma_i = \sum_{j=1}^{n} A_j P_j(x_i) = [P]\{A\}$$

- **So we devised a simple model uncertainty based on the uncertainty in *n*** ∂n
  - Just by looking at neighboring fit orders

A big improvement





Prime, M. B., and Hill, M. R., 2006, "Uncertainty, Model Error, and Order Selection for Series-Expanded, Residual-Stress Inverse Solutions," *Journal of Engineering Materials and Technology*, **128**(2), pp. 175-185.

- **Looking at the easy part of uncertainty, like the strain errors, is not good enough**

- **Often the bigger error is *not* the measurement but is the *model* we use to describe our physical system**
  - Model error

- **With some effort, we can find ways to improve the uncertainty estimate for processed data**

- **Least squares fits are a great way to use more data to get a better answer**
  - But can give very low uncertainty estimates using simple propagation
  - Because errors often do not fit the model

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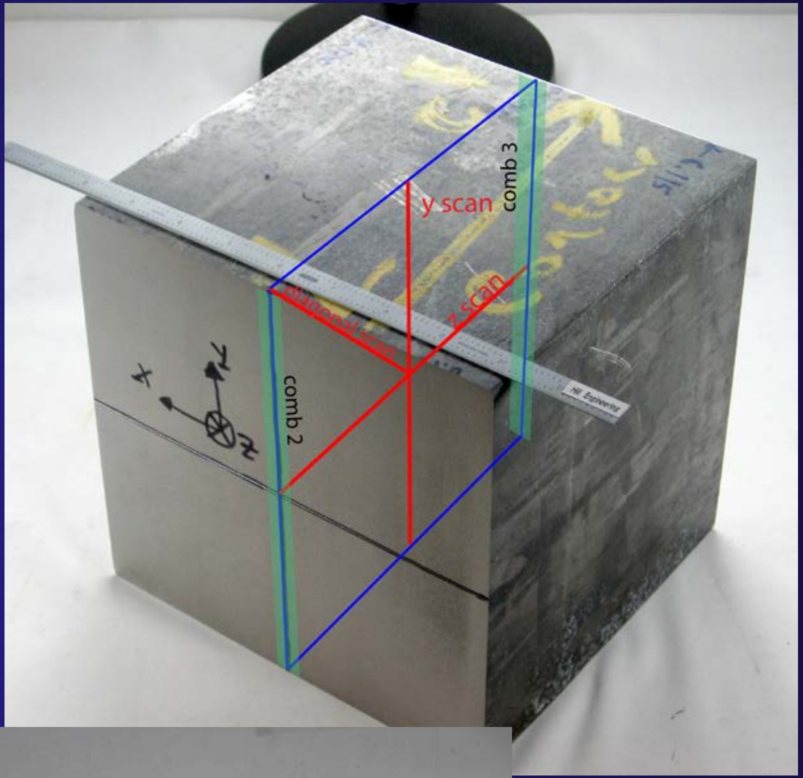
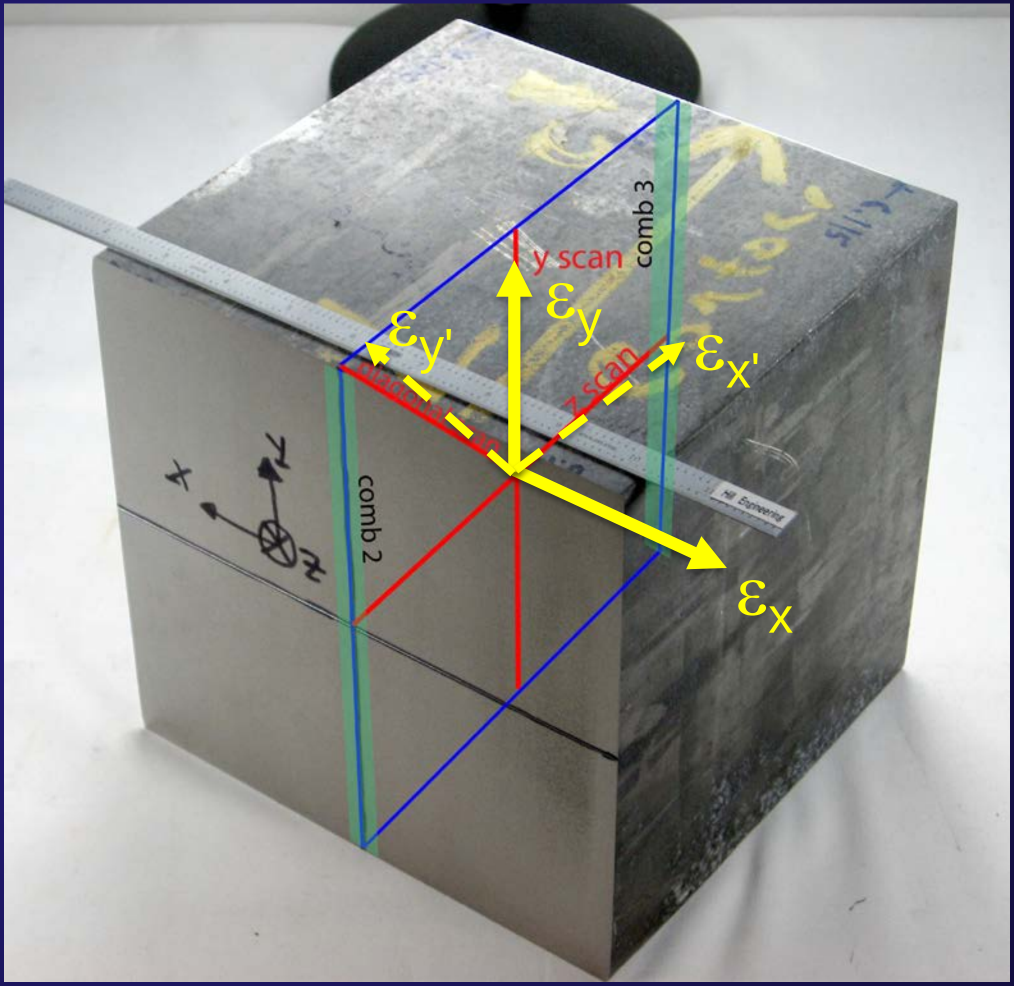
State-of-the-art neutron diffraction stress mapping on large forging

- **7050 Aluminum forging**
  - NOT stress relieved
  - ≈ 200 mm × 200 mm × 200 mm section
- **Time-of-flight diffraction at SMARTS at LANL**
  - Rietveld refinement to get strains
- **Low penetration on this thick part**
  - So used 3 scan lines to get a reasonable map over cross-section
  - Big sampling volume
    - 5 x 5 mm slits
    - 4 mm collimators
  - Took ~ 120 hours
- **Used combs to get stress-free reference (d0)**

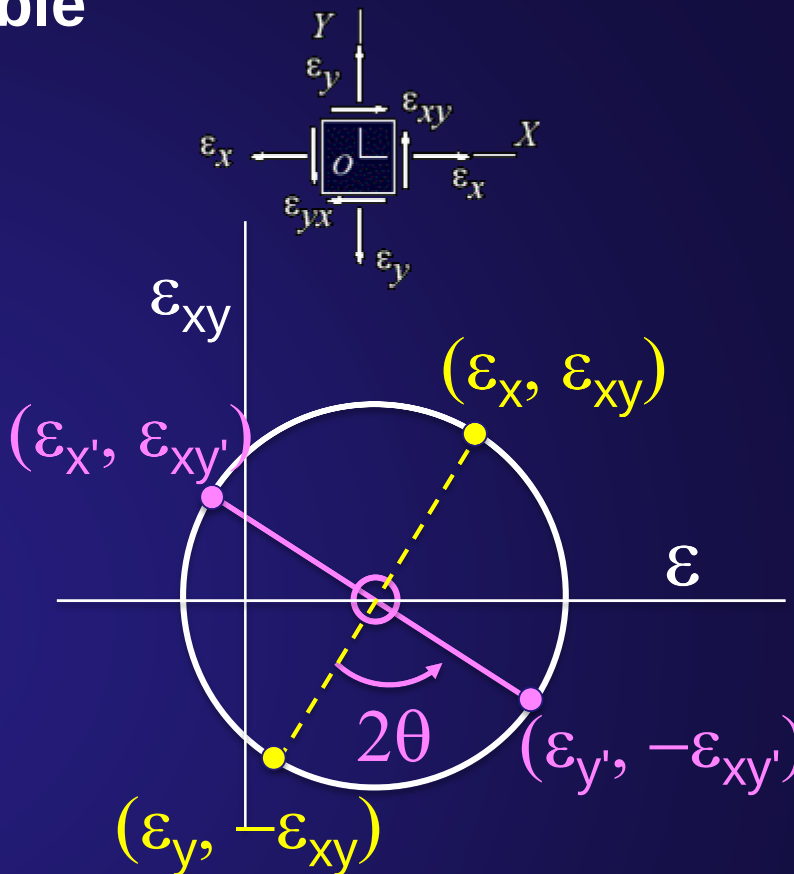


Additional neutron orientation to get ε_{xy} , τ_{xy}

- **As is standard, used two orientations to get 3 ε's and therefore σ in *x-y-z* directions**
- **We were also interested in *x-y* shear stresses**
  - So added an orientation at 45° in *x-y* plane



Redundant data gives an inviolable check on correctness of results

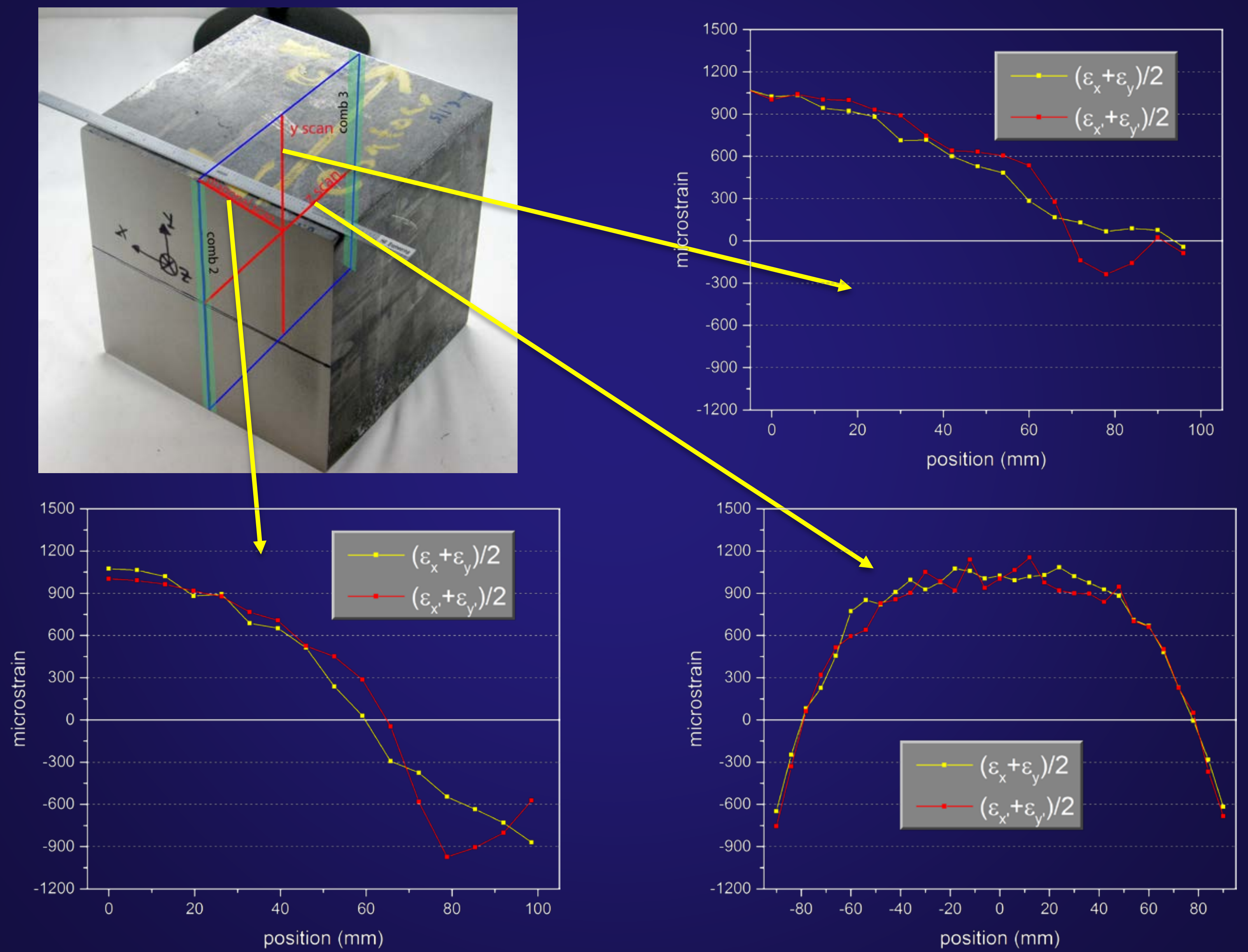


- **We have redundant information**
  - It only takes three in-plane strains to determine the whole in-plane strain state
  - We have 4
- **Mohr's circle is a convenient graphic construct of in-plane strains**
- **Can be used to rotate strain state**
- **Gives an easy consistency check:**
  - The center of the circle is always the same

$$\frac{\varepsilon_x + \varepsilon_y}{2} = \frac{\varepsilon_{x'} + \varepsilon_{y'}}{2}$$

  - (rotational invariant)

How good should this agreement be?

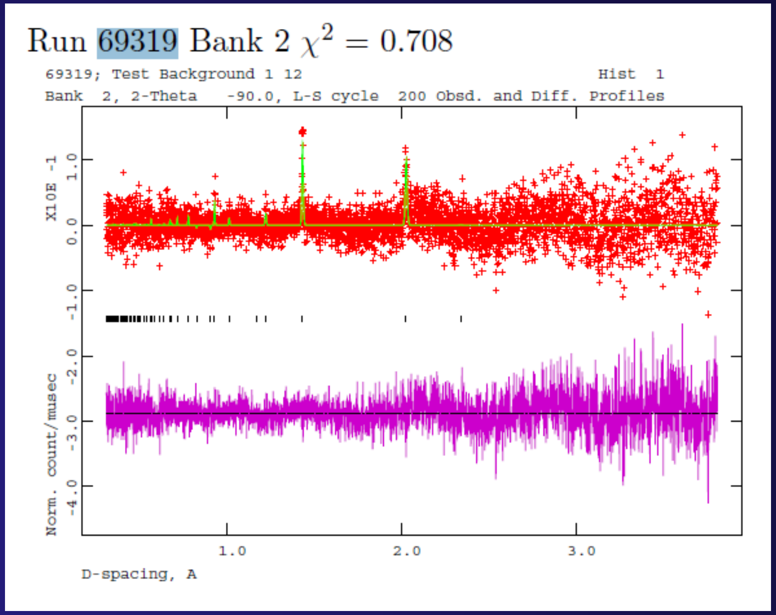


Standard Neutron Uncertainty Calculation uses Uncertainty in Peak Fit

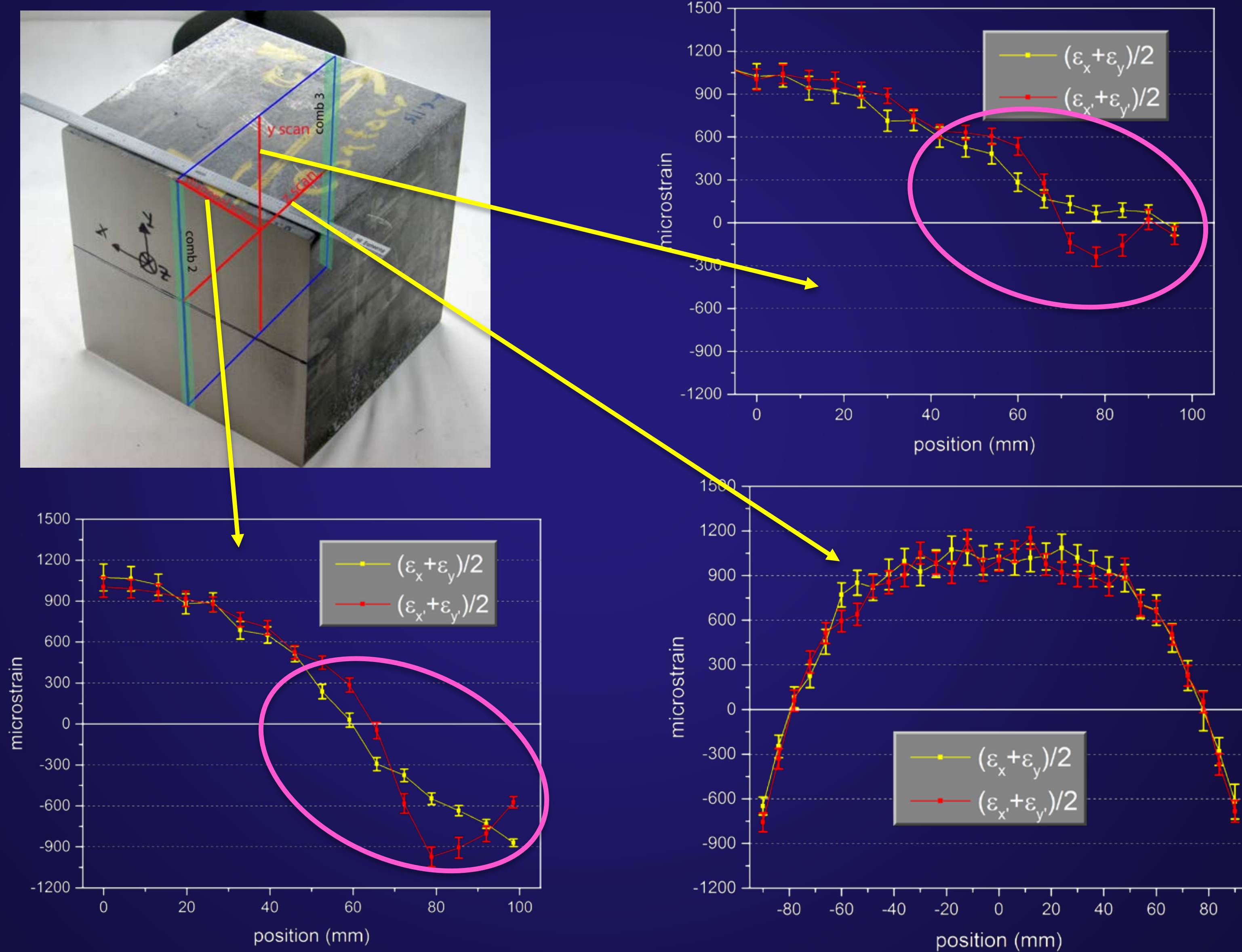
- **Rietveld refinement fits diffraction peak pattern to fcc crystal structure of aluminum to give lattice parameter and uncertainty**
  - $a \pm \delta a$
- **Which we can propagate through all equations**
  - $\varepsilon = \frac{a - a_0}{a_0}$ uncertainty on a AND a_0

$$\sigma_i = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}\left[\varepsilon_i + \frac{\nu}{1+\nu}(\varepsilon_j + \varepsilon_k)\right]$$

  - To get $\sigma \pm \delta\sigma$
- ***** I added extra uncertainty to a_0 because of uncertainty in spatial variation (which was measured)**



In some regions, uncertainties are underestimated, almost by definition



Can we independently check the accuracy of the neutron results?

- **The neutron measurements were motivated as a independent validation of fracture surface contour measurement**
  - Spoke on this in Summit 2013

- **But maybe we can learn something about the neutron accuracy with the comparison**

- **Contour/fracture uncertainties calculated based on**
  - Olson, M. D., DeWald, A. T., Prime, M. B., and Hill, M. R., 2015, "Estimation of Uncertainty for Contour Method Residual Stress Measurements," *Experimental Mechanics*, **55**(3), pp. 577-585.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Forensic determination of residual stresses and K_I from fracture surface mismatch

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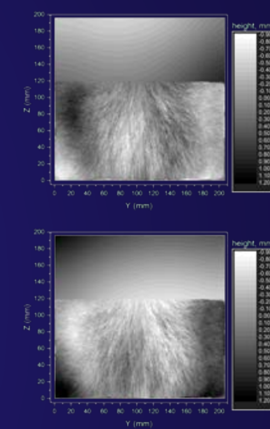
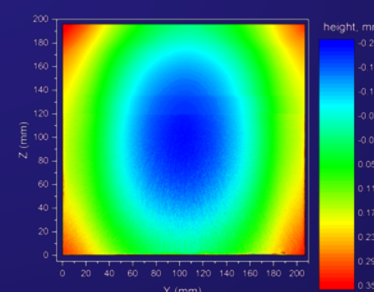
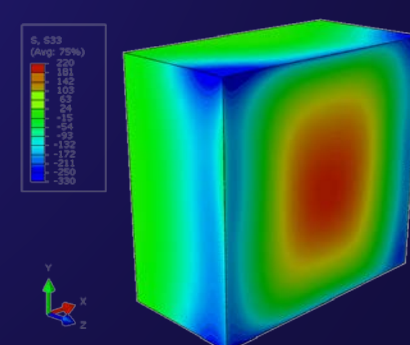
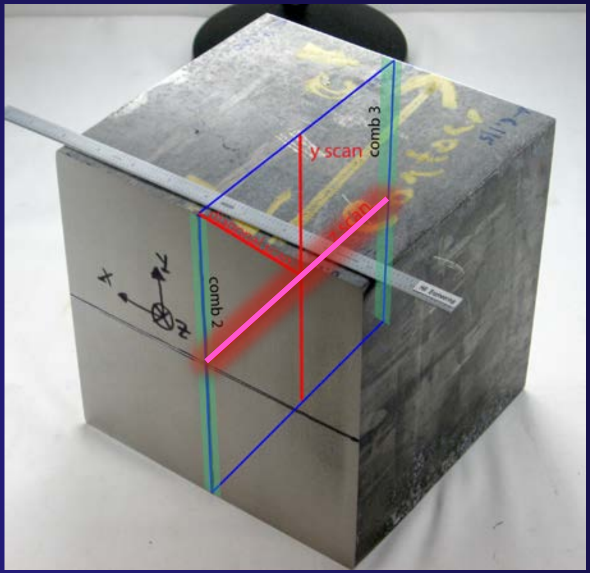


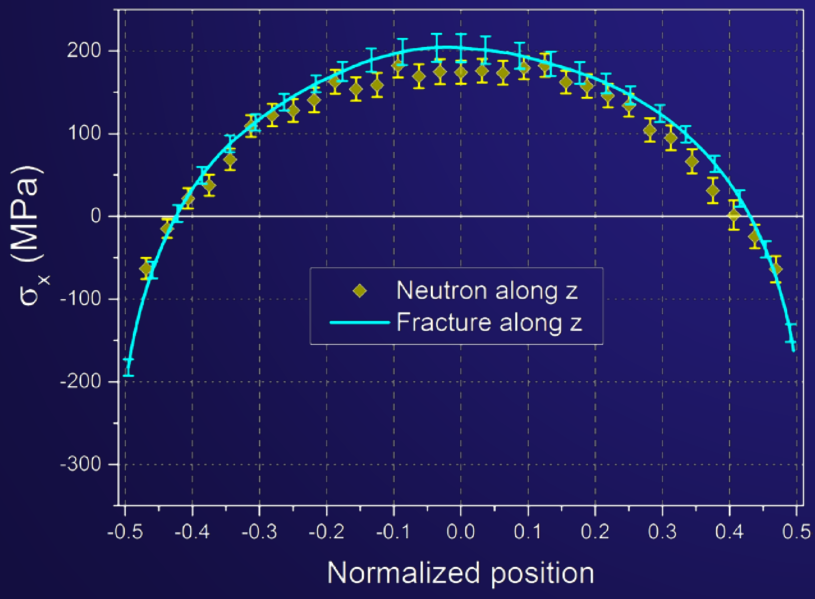


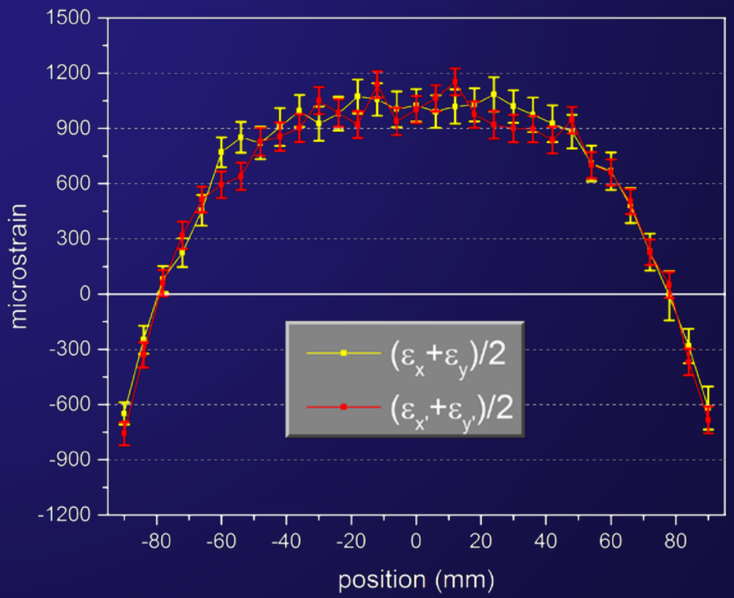


Z-scan neutron uncertainties look OK

- **Neutron and fracture-surface-contour results agree within uncertainty**
- **And this is scan where strain consistency check also passed within uncertainty**
- **Interestingly, region near *z*=0 where ε's barely passed had biggest disagreement**
  - Could be a_0 bias error
  - Could probably use a bigger uncertainty

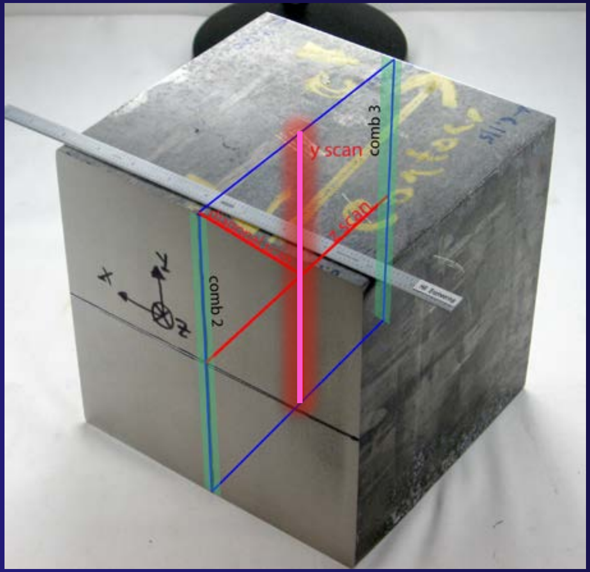


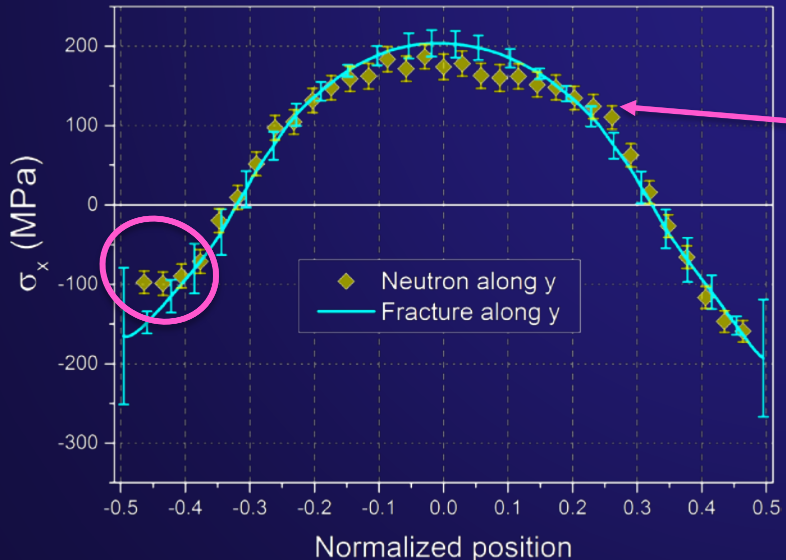


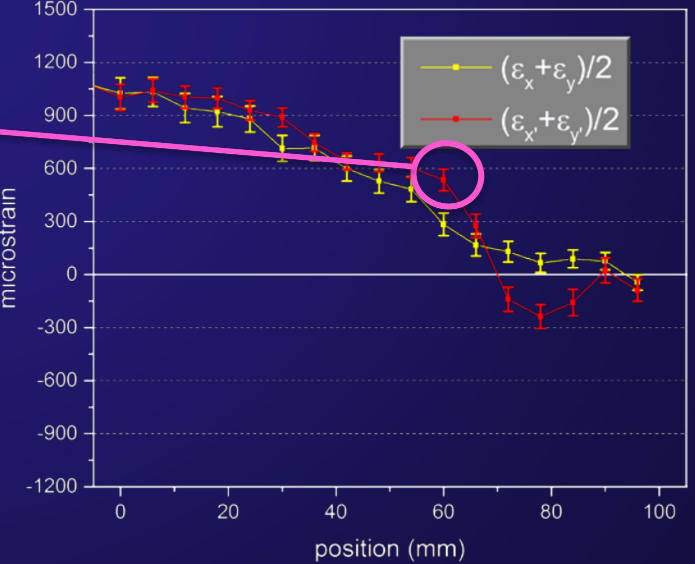


Y-scan neutron uncertainties underestimated in places

- **Uncertainties underestimated sometimes**
  - Correlates well with strain checks inconsistency
  - Even if some places with consistency have good agreement
- **Note; if I had not added additional uncertainty to *a_0*, neutron error bars would be even smaller**

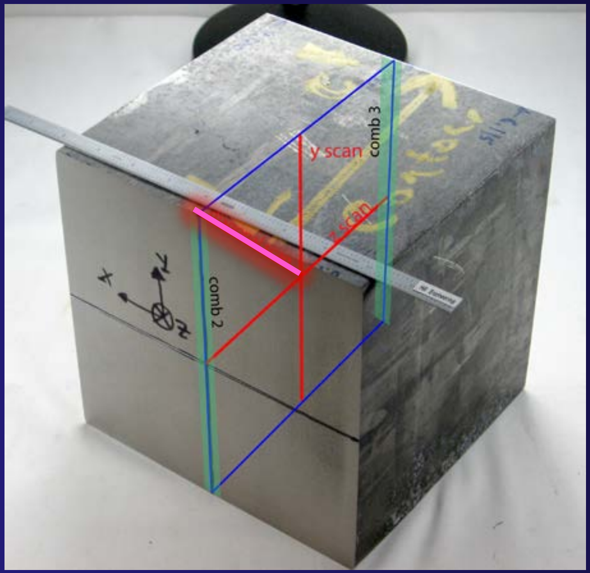


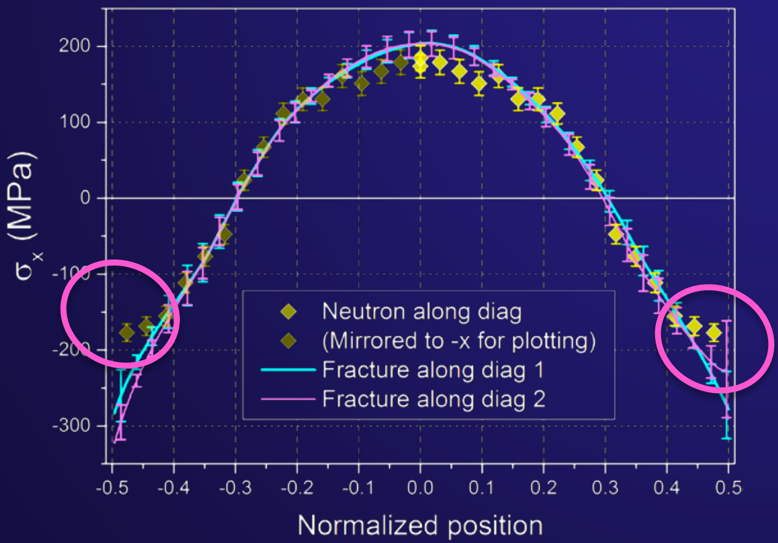


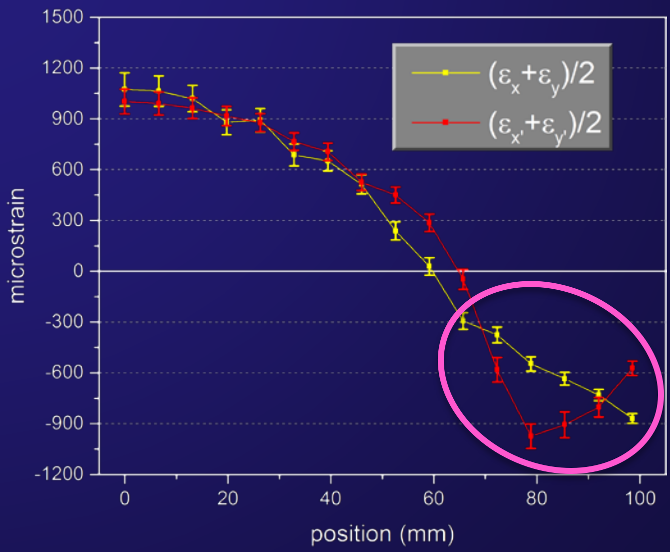


Diagonal scan neutron uncertainties

- **More correlation between strain check inconsistency and disagreement between methods**

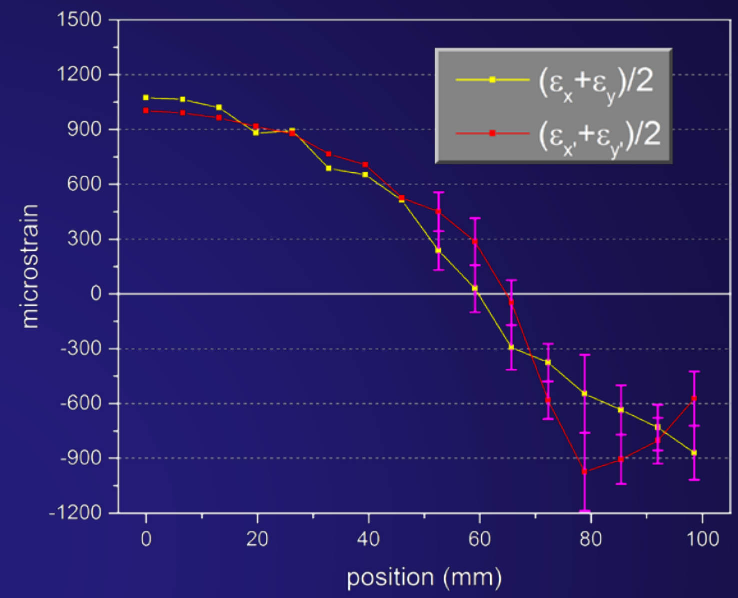


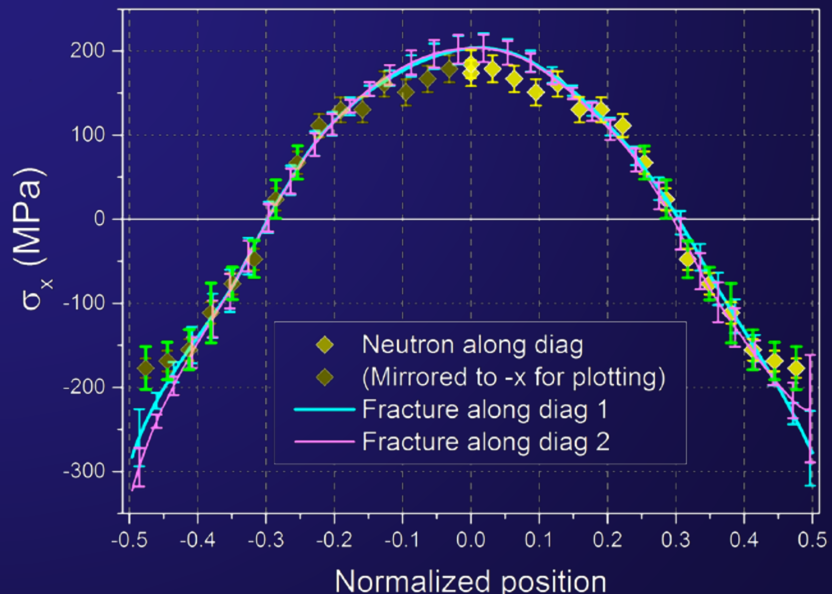




One simple improvement

- **Set strain uncertainty to the *larger* of**
  - Conventionally propagated uncertainty
  - ½ the difference in the consistency check
- **Gives us a much better uncertainty estimate for this test**
  - based on comparison to fracture surface results





Is this a practical approach?

Can we use this redundant data idea generally with neutron diffraction?

- **Requires at least one extra orientation in order to get a redundant strain**
  - Would be a 50% increase compared to usual two orientations
  - Except that you could probably get away with not doing every measurement point

- **Redundant orientations are rare, and not used this way**
  - A least squares fit is used to get a more accurate strain state - good
  - With a lower uncertainty based on the least squares fit
    - Bad if the uncertainty is less than the consistency discrepancy

Conclusions

- **Standard uncertainty propagation underestimates uncertainty more often than not**
- **Measurement providers can do several things to improve uncertainty estimates**
  - Data driven
    - Take redundant data in order to check and if necessary increase uncertainties
    - Repeat measurements to establish repeatability-based uncertainty
    - Multiple method comparisons
    - Repeat measurements with changes
      - Contour cut in other direction
      - Different diffraction peak
  - Analysis
    - Include more uncertainty sources in error propagation
    - Include alternate uncertainty estimates
- **Users can also contribute**
  - Insist on documented uncertainty estimate
    - But you have to pay for it
  - Support repeats and other studies to better establish uncertainty