

Material model inference from experimental data

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Overview

- Bayesian analysis
 - ▶ appropriate for analyzing physics experiments
- Likelihood analysis
 - ▶ relation to chi-squared
 - ▶ estimation of parameters and their uncertainties
- Material characterization experiments
- Data analysis using Zerilli-Armstrong model
 - ▶ difficulties in matching data
 - ▶ importance of expertise to obtain satisfactory result
 - ▶ systematic effects, uncertainties

Acknowledgments

Collaborators

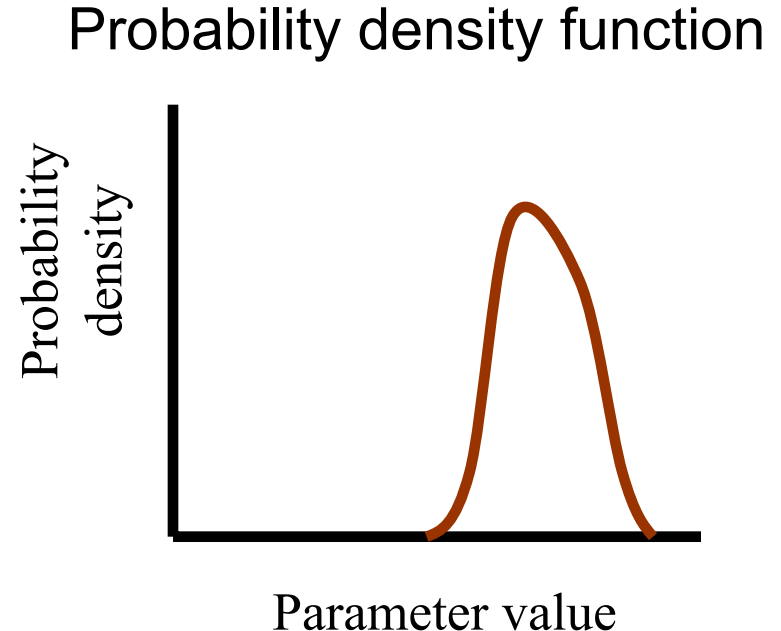
- Shuh-Rong Chen, MST-8
- François Hemez, ESA-WR

Discussions

- Larry Hull, Eric Ferm, DX-3
- Chris Romero, Tom Duffy, DX-7
- Paul Maudlin, T-3
- Mark Anderson, ESA-WR
- Kathy Campbell, Mike McKay, Dave Higdon,
Alyson Wilson, Mike Hamada, D-1
- Tom Dey, X-7

Uncertainties and probabilities

- Uncertainties in parameters are characterized by probability density functions (pdf)
- Probability interpreted as quantitative measure of “**degree of belief**”
- This interpretation sometimes referred to as “subjective probability”
- Rules of classical probability theory apply



Bayesian analysis of experimental data

- Bayesian approach
 - ▶ focus is as much on uncertainties in parameters as on their best (estimated) value
 - ▶ appropriate for Uncertainty Quantification (UQ)
 - ▶ use of prior knowledge, e.g., previous experiments, modeling expertise, subjective
 - ▶ model checking –
 - does model agree with experimental evidence?
 - ▶ compatible with scientific method
- Goal is estimation of **model parameters and their uncertainties**

Bayesian analysis of experimental data

- Bayes theorem

$$p(\mathbf{a} \mid \mathbf{d}, I) \propto p(\mathbf{d} \mid \mathbf{a}, I) p(\mathbf{a} \mid I)$$

- ▶ where

\mathbf{d} is the vector of measured data values

\mathbf{a} is the vector of parameters for model that predicts the data

- ▶ $p(\mathbf{d} \mid \mathbf{a}, I)$ is called the **likelihood** (of the data given the true model and its parameters)
- ▶ $p(\mathbf{a} \mid I)$ is called the **prior** (on the parameters \mathbf{a})
- ▶ $p(\mathbf{a} \mid \mathbf{d}, I)$ is called the **posterior** – fully describes uncertainty in the parameters
- ▶ I stands for whatever **background information** we have about the situation, results from previous experience, our expertise, and the model used

Bayesian analysis – role of the prior

- The prior in Bayes theorem distinguishes Bayesian analysis from “traditional” frequentist statistics
- The prior can be chosen to be non-informative
 - ▶ examples: uniform, uniform in log, maximum entropy
 - ▶ to reflect complete lack of knowledge about situation, to avoid biasing result
 - ▶ to be objective(?); often appropriate for physics analyses
- The prior can be chosen to be informative
 - ▶ to enforce physical constraints, e.g., nonnegativity (density)
 - ▶ to incorporate information from previous experiments
 - ▶ to reflect expert knowledge (elicitation process)
- Choice of prior is subject to discussion and review

The model and parameter inference

- We write the model as

$$y = y(\mathbf{x}, \mathbf{a})$$

- ▶ where y is a physical quantity, which is modeled as a function of the independent variables vector \mathbf{x} and \mathbf{a} represents the model parameters vector
- In inference, the aim is to determine:
 - ▶ the parameters \mathbf{a} from a set of n measurements d_i of y under specified conditions x_i
 - ▶ and the uncertainties in the parameter values
- This process is called parameter inference, model fitting (or regression) but often uncertainty analysis not done, as in parameter estimation

The likelihood and chi-squared

- The form of the likelihood $p(\mathbf{d} | \mathbf{a}, I)$ depends on how we model the uncertainties in the measurements \mathbf{d} .
- Assuming the error in each measurement d_i is normally (Gaussian) distributed with zero mean and variance σ_i^2 , and that the errors are statistically independent,

$$p(\mathbf{d} | \mathbf{a}) \propto \prod_i \exp\left[-\frac{[d_i - y_i(\mathbf{a})]^2}{2\sigma_i^2}\right]$$

where y_i is the value predicted for parameter set \mathbf{a}

- The above exponent is related to chi squared

$$\chi^2 = -2 \log[p(\mathbf{d} | \mathbf{a})] = \sum_i \left[\frac{[d_i - y_i(\mathbf{a})]^2}{\sigma_i^2} \right]$$

- For this error model, likelihood is $p(\mathbf{d} | \mathbf{a}) \propto \exp(-\frac{1}{2} \chi^2)$

Likelihood analysis

- For a non-informative **flat prior**, the posterior is proportional to the likelihood
- Given the relationship between chi-squared and the likelihood, the posterior is

$$p(\mathbf{a} | \mathbf{d}) \propto p(\mathbf{d} | \mathbf{a}) \propto \exp\left(-\frac{1}{2} \chi^2\right)$$

- Thus, parameter estimation based on **maximum likelihood** is equivalent to that based on **minimum chi squared**

Characterization of chi-squared

- Expand vector \mathbf{y} around \mathbf{y}^0 :

$$y_i = y_i(x_i, \mathbf{a}) = y_i^0 + \sum_j \frac{\partial y_i}{\partial a_j} \Big|_{\mathbf{a}^0} (a_j - a_j^0) + \dots$$

- The derivative matrix is called the *Jacobian*, \mathbf{J}
- Estimated parameters $\hat{\mathbf{a}}$ minimize χ^2 (MAP estimate)
- As a function of \mathbf{a} , χ^2 is quadratic in $\mathbf{a} - \hat{\mathbf{a}}$

$$\chi^2(\mathbf{a}) = \frac{1}{2}(\mathbf{a} - \hat{\mathbf{a}})^T \mathbf{K} (\mathbf{a} - \hat{\mathbf{a}}) + \chi^2(\hat{\mathbf{a}})$$

where \mathbf{K} is the curvature matrix (aka the *Hessian*);

$$[\mathbf{K}]_{jk} = \frac{\partial^2 \chi^2}{\partial a_j \partial a_k} \Big|_{\hat{\mathbf{a}}} = \mathbf{J} \mathbf{\Lambda} \mathbf{J}^T \quad ; \quad \mathbf{\Lambda} = \text{diag}(\sigma_1^{-2}, \sigma_2^{-2}, \sigma_3^{-2}, \dots)$$

Parameter inference

- Posterior $p(\mathbf{a} | \mathbf{d}, I)$ can be written as

$$p(\mathbf{a} | \mathbf{d}) = \frac{1}{\det[\mathbf{C}] (2\pi)^{n/2}} \exp\left[-\frac{1}{2}(\mathbf{a} - \hat{\mathbf{a}})^T \mathbf{C}^{-1} (\mathbf{a} - \hat{\mathbf{a}})\right]$$

- From known properties of Gaussian distribution, covariance matrix for parameter uncertainties is

$$\text{cov}(\mathbf{a}) = \left\langle (\mathbf{a} - \hat{\mathbf{a}})(\mathbf{a} - \hat{\mathbf{a}})^T \right\rangle \equiv \mathbf{C} = 2\mathbf{K}^{-1}$$

- Thus, the chi-squared functionality provides the basis for inference about parameters \mathbf{a}
- Recall assumptions:
 - ▶ linearized model holds for measured quantities ($y = f(\mathbf{x}, \mathbf{a})$)
 - ▶ meas. errors indep. & Gaussian distrib. with known variance
 - ▶ uniform prior on parameters \mathbf{a}

Model checking – goodness of fit

- Chi-squared analysis is based on assumption that measurement errors Gaussian distributed, independent
- After minimum χ^2 is found, one can check whether the value of χ^2 is consistent with that assumption
- Chi-squared distribution table gives probability p for obtaining the observed χ^2 value or higher
- Reduced chi-squared is χ^2/ν , where ν is
degrees of freedom = # data – # parameters
- Property of χ^2 distribution: $p = 50\%$ is near $\chi^2/\nu = 1$
- Checks self-consistency of models used to explain data (weakly)

Model checking – goodness of fit

- Check of chi-squared value only weakly confirms validity of models used
- Chi-squared value depends on numerous factors:
 - ▶ assumption that errors follow Gaussian distribution and are statistically independent
 - ▶ proper assignment of standard deviation of errors
 - ▶ correctness of model used to calculate measured quantity
 - ▶ measurements correspond to calculated quantity (proper measurement model)
- Thus, a reasonable chi-squared p value does not necessarily mean everything is OK, because there may be compensating effects

Analysis of multiple data sets

- To combine the data from multiple, independent data sets into a single analysis, the combined likelihood is

$$p_{all}(\mathbf{d} | \mathbf{a}) \propto \prod_k p(\mathbf{d}_k | \mathbf{a})$$

where $p(\mathbf{d}_k | \mathbf{a}, I)$ is likelihood from k th data set

- ▶ assumes the uncertainties in different data sets are statistically independent
- Thus, because $\chi^2 = -2 \log [p(\mathbf{d} | \mathbf{a})]$, just add χ^2 s from each data set

$$\chi_{all}^2 = \sum_k \chi_k^2$$

Inclusion of Gaussian priors

- To include priors, use Bayes theorem

$$p(\mathbf{a} | \mathbf{d}, I) \propto p(\mathbf{d} | \mathbf{a}, I) p(\mathbf{a} | I)$$

- For a Gaussian prior on a parameter a

$$p(a | I) = \frac{1}{\sigma_a (2\pi)^{1/2}} \exp\left[-\frac{(a - \tilde{a})^2}{2\sigma_a^2}\right]$$

where \tilde{a} is the default value for a and σ_a^2 is the assumed variance

- The minus-log-posterior for the parameter a is

$$-\log p(a | \mathbf{d}, I) = \varphi(a) = \frac{1}{2} \chi^2 + \frac{(a - \tilde{a})^2}{2\sigma_a^2}$$

Motivating example

- Problem statement
 - ▶ design containment vessel using high-strength steel, HSLA 100
 - ▶ one design criterion relates to wall penetration by schrapnel
 - ▶ predict degree of wall penetration by specified projectile
 - ▶ estimate uncertainty in this prediction to estimate safety factor
- Our present goal is to determine for HSLA 100 the parameters and their uncertainties for the Zerilli-Armstrong plastic strength model for
 - ▶ strains up to fracture for use at
 - ▶ room temperature
 - ▶ high strain rates
- These conditions match the intended application

HSLA 100

- Material under study is the high-strength, low-alloy steel designated as HSLA 100
 - ▶ used in critical structural applications
- Manufacture of this steel is done under tight specifications
 - ▶ composition is certified and uniform
 - ▶ properties should be quite reproducible
- For most metals, processing can affect properties of the material
 - ▶ processing often involves rolling of billets into sheets and subsequent heat treatment

Stress-strain relation for plastic deformation

- Zerilli-Armstrong model describes strain rate- and temperature-dependent plasticity in terms of stress σ (or s) as function of plastic strain ε_p

$$\sigma = \alpha_1 + \alpha_5 \varepsilon_p^{\alpha_6} + \alpha_2 \exp \left[\left(-\alpha_3 + \alpha_4 \log \frac{\partial \varepsilon_p}{\partial t} \right) T \right]$$

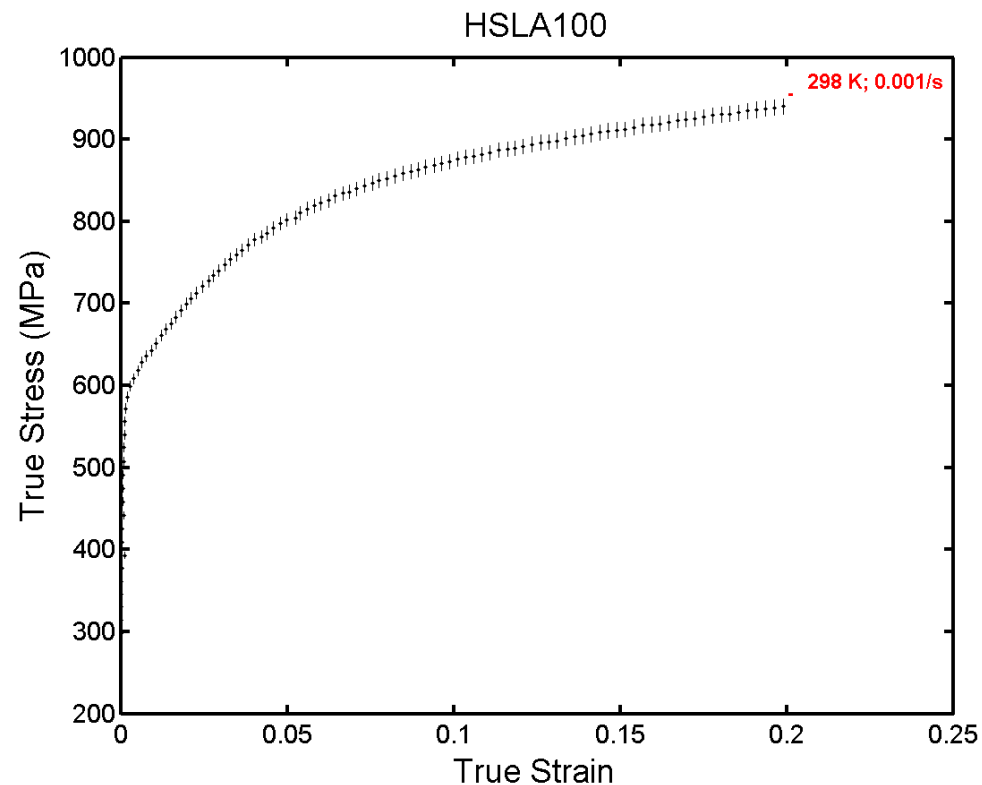
- Six parameters -
 - ▶ 2 parameters (α_5 & α_6) specify dependence of stress on strain
 - ▶ 4 remaining parameters specify additive offset as function of temperature and strain rate
- Z-A formula based on dislocation mechanics model
 - ▶ may not hold for all experimental conditions

Material characterization experiments

- Quasi-static experiments
 - ▶ subject material specimen to tension or compression
 - ▶ measure force and corresponding sample length
 - ▶ convert to true stress and true strain
- Hopkinson-bar experiments
 - ▶ send shock wave into thin disc of material
 - ▶ measure length of specimen as a function of time
 - ▶ interpret in terms of true stress and true strain at a calculated strain rate using simulation code
 - ▶ correct measured temperature of specimen for work done on sample, assuming adiabatic process

Quasi-static experiments

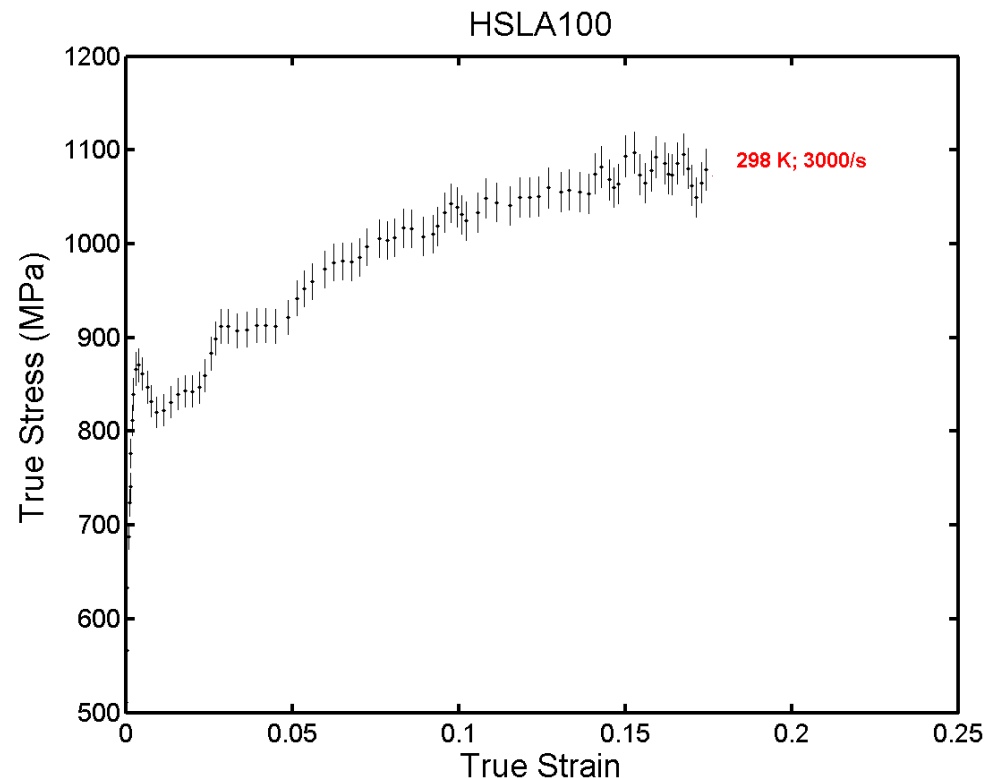
- Data from quasi-static compression experiments tend to be of high quality
- Systematic uncertainties in the basic measurements should be very small
- Example shows data at room temperature
 - ▶ elastic region
 - ▶ yield stress
 - ▶ plastic region
- Error bars shown are 1% or ~ 10 Mpa
 - ▶ error bars seem too large!
 - ▶ but experience dictates caution



†data supplied by S-R Chen, MST-8

Hopkinson-bar experiments

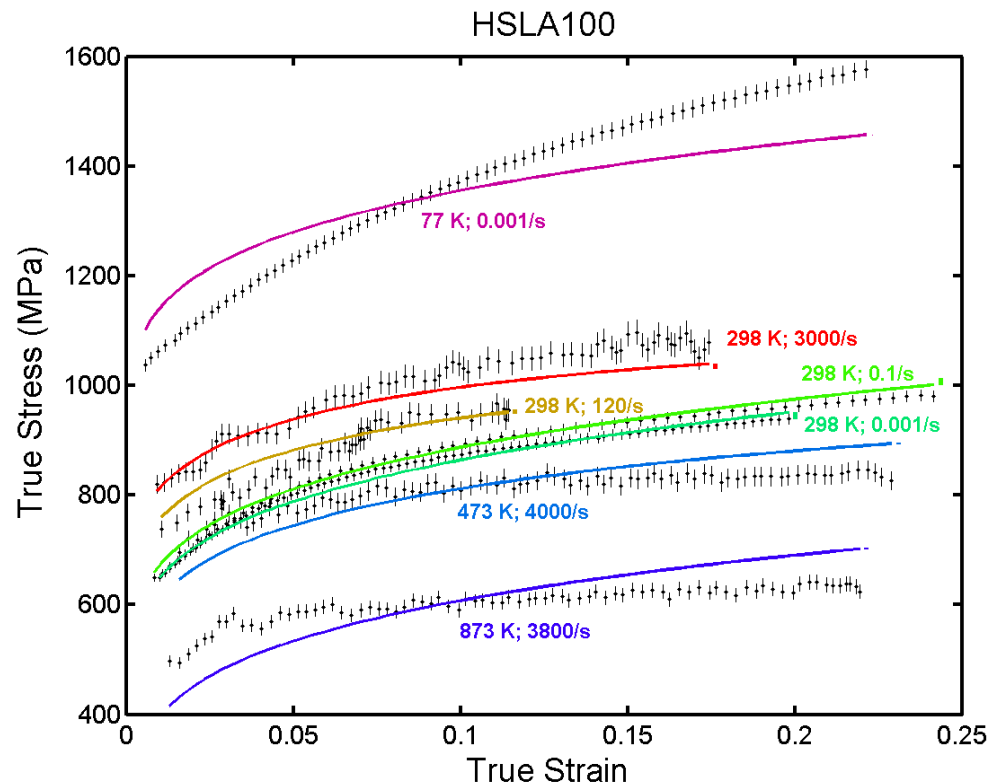
- Data from Hopkinson-bar experiments tend to be of medium quality
- Systematic uncertainties in the basic measurements should be small
- Observe artifacts in the data
 - ▶ arise from reflected shocks
 - ▶ should exclude these
- Must rely on simulation code to calculate strain rate
- Error bars shown are 2% or ~20 MPa
 - ▶ plausible uncertainty level



†data supplied by S-R Chen, MST-8

Fit ZA model to all data

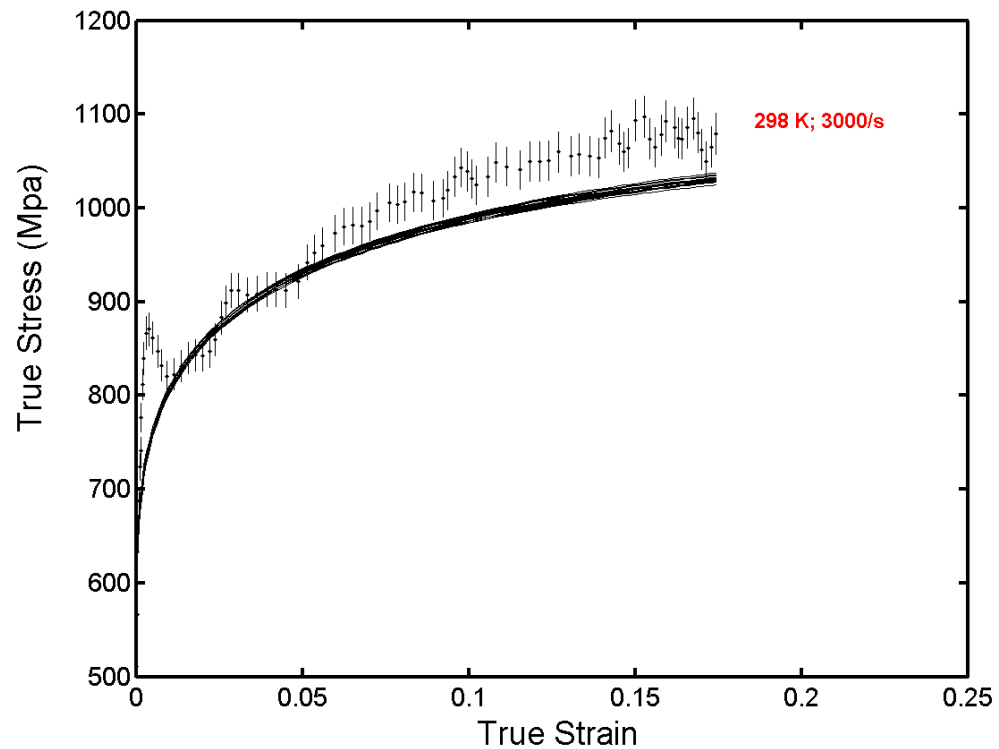
- 7 data sets at various strain rates and temperatures
- Fit to all data above elastic region or after first bump in Hopkinson-bar data
- Model does not reproduce stress-strain curves at high and low temperatures
- Fit is far from expt. measurements for target conditions of room temp., high strain rate
- Uncertainties are highly correlated



† data supplied by S-R Chen, MST-8

Monte Carlo sampling from posterior

- Use Monte Carlo technique to draw random ZA parameter vectors from their uncertainty distribution
- Plot corresponding curves for room temperature, high strain rate and compare to measurements
- Conclude that the parameters inferred from last slide do not plausibly represent the data for target conditions

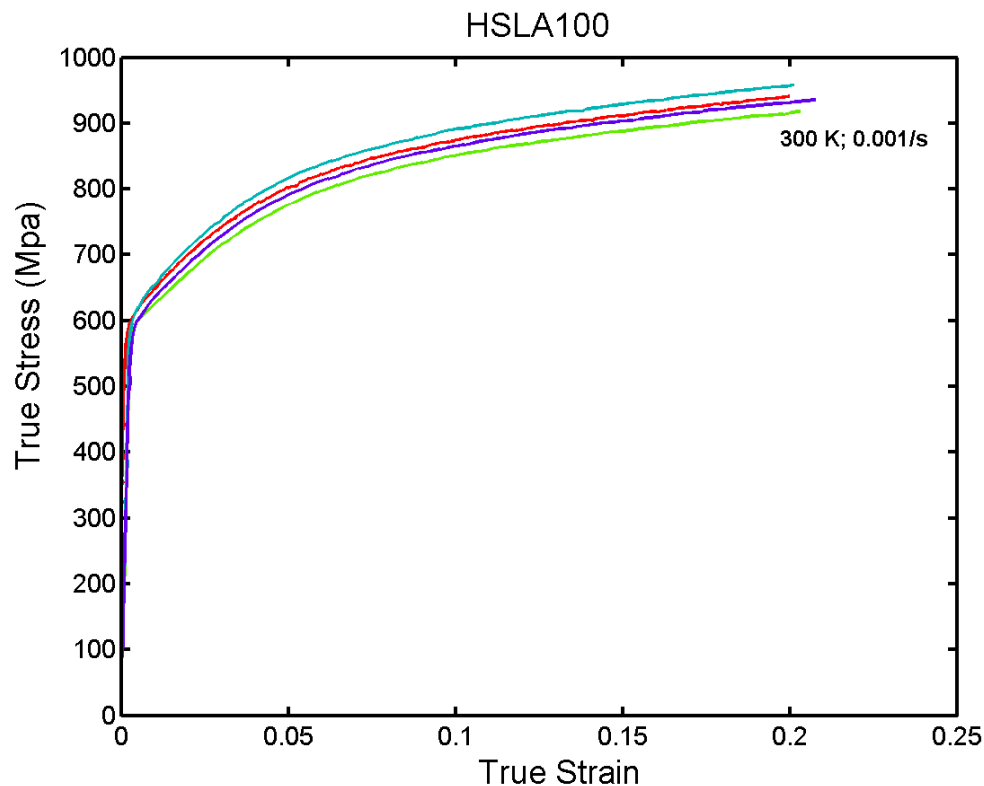


Refine analysis to accommodate data

- Need to improve analysis for intended operating conditions (moderate strain, high strain rate, and room temperature)
- Approach is
 - ▶ limit the data for high and low temps to low strain region (<0.06); reasoning is that dislocation mechanics behavior at high strain values is clearly different than at room temperature, but would like to capture behavior near yield points.
 - ▶ can not just ignore these data – they are needed to determine temp and strain rate dependence in ZA model
 - ▶ strain rate dependence seen in experimental data do not conform with ZA model, or any other smoothly varying model
 - ▶ inclusion of sample-to-sample uncertainties into analysis accommodates these differences
 - ▶ treat sample-to-sample variability as systematic uncertainty

Repeated experiments

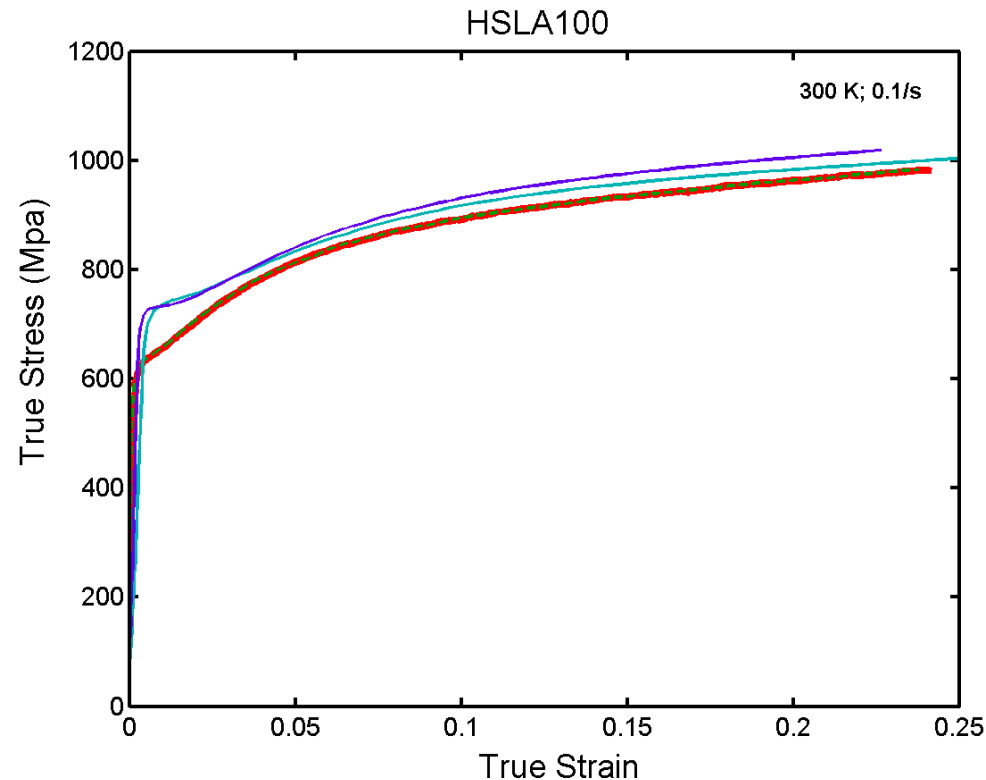
- Repeated experiments
 - ▶ stability of apparatus
 - ▶ indication of random component of error
 - ▶ may or may not indicate systematic error
- Figure shows curves obtained from four samples taken from random positions in thick plate
- Sample-to-sample rms deviation is around 20 MPa at strain of 0.1
- Treat this variability as **systematic uncertainty**



†data supplied by S-R Chen, MST-8

Repeated experiments

- Figure shows curves from four samples
 - ▶ nearly identical response for two taken from nearby position and tested together (red and green dashed lines)
 - ▶ but disagree with previous tests on samples from different stock, perhaps caused by different processing
- Observe sample-to-sample differences of around 20 MPa for strains > 0.03
- Treat this variability as **systematic uncertainty**



† data supplied by S-R Chen, MST-8

Types of uncertainties in measurements

- Two major types of errors
 - ▶ random error – different for each measurement
 - in repeated measurements, get different answer each time
 - often assumed to be statistically independent, but often aren't
 - ▶ systematic error – same for each measurement within a group
 - component of measurements that remains unchanged
 - for example, caused by error in calibration or zeroing
- Nomenclature varies
 - ▶ physics – random error and systematic error
 - ▶ statistics – random and bias
 - ▶ metrology standards (NIST, ASME, ISO) – random and systematic uncertainties (now)

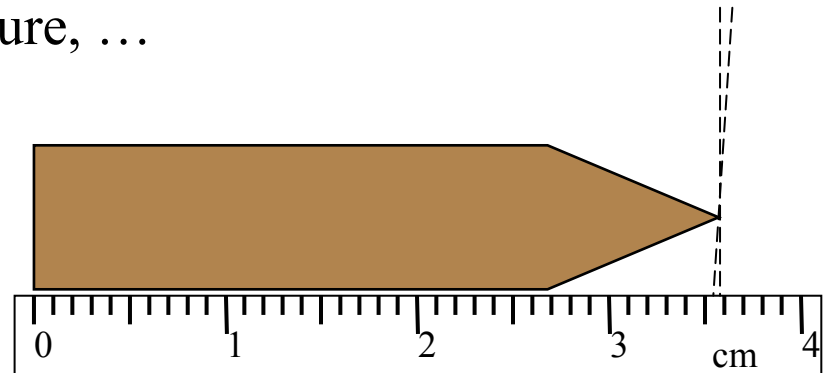
Types of uncertainties in measurements

- Simple example – measurement of length of a pencil
 - ▶ random error
 - interpolation between ruler tick marks
 - ▶ systematic error
 - accuracy of ruler's calibration; manufacturing defect, temperature, ...

- Parallax

- ▶ reading depends on how person lines up pencil tip
- ▶ random or systematic error?

depends on whether measurements always made by same person in the same way or made by different people

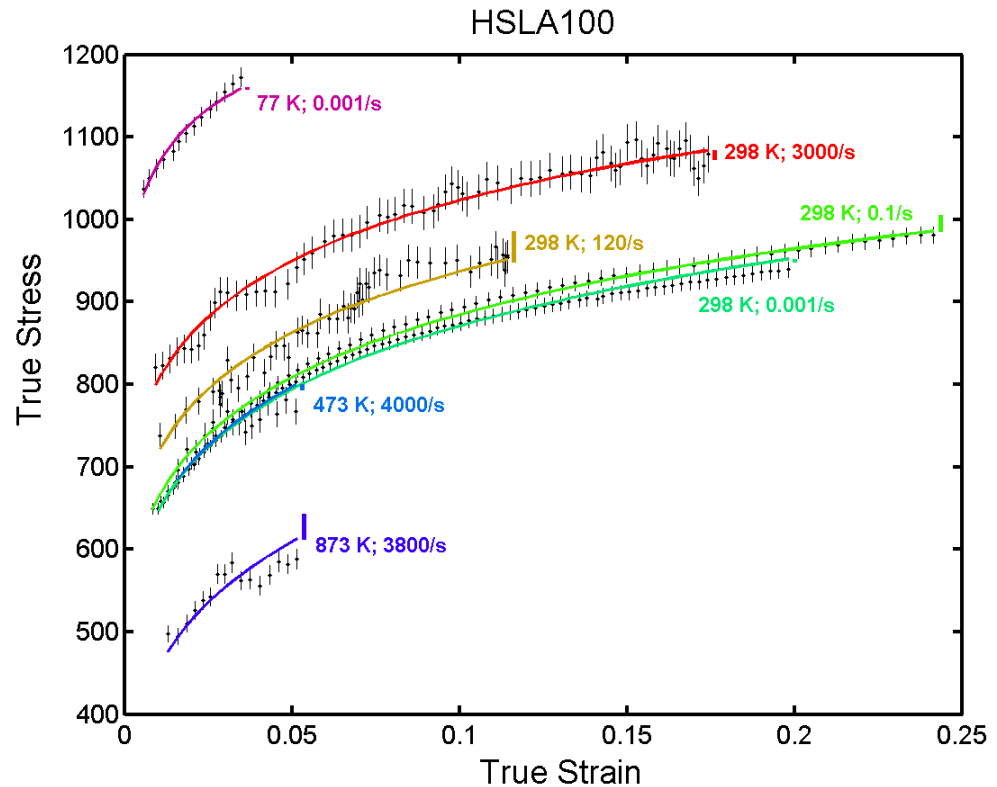


Include offsets for each data set

- Represent offset of k th data set with a parameter Δ_k
- Treat offset as **systematic effect** for each curve, but as random effect when combining curves
- Include what we know about Δ_k in terms of a prior
 - ▶ assume Gaussian distribution
 - ▶ assume most probable value of Δ_k is zero and that uncertainty distribution has an rms deviation of σ_k
- Then, the posterior is
$$-\log p(\mathbf{a} | \mathbf{d}, I) = \varphi(\mathbf{a}) = \frac{1}{2} \sum_k \chi_k^2 + \frac{1}{2} \sum_k \frac{\Delta_k^2}{\sigma_k^2}$$
- For HSLA 100 analysis, we have 7 data sets and ZA model has 6 parameters; thus 13 variables in fit

Fit ZA model to selected data

- Use data above elastic region or after first bump in Hopkinson-bar data
- Additionally, restrict data at high and low temps. to low strain (near yield point)
- Add offset parameter for each curve to represent **sample-to-sample variation**
- Fit reasonably represents data for target conditions of room temp., high strain rate



† data supplied by S-R Chen, MST-8

Fit ZA model to selected data

- Results summarized by
 - ▶ estimated parameter values
 - ▶ estimated rms errors
 - ▶ correlation matrix
- **All of these are necessary to fully specify parameters and their uncertainties**

Parameters and their standard errors (CGS units)

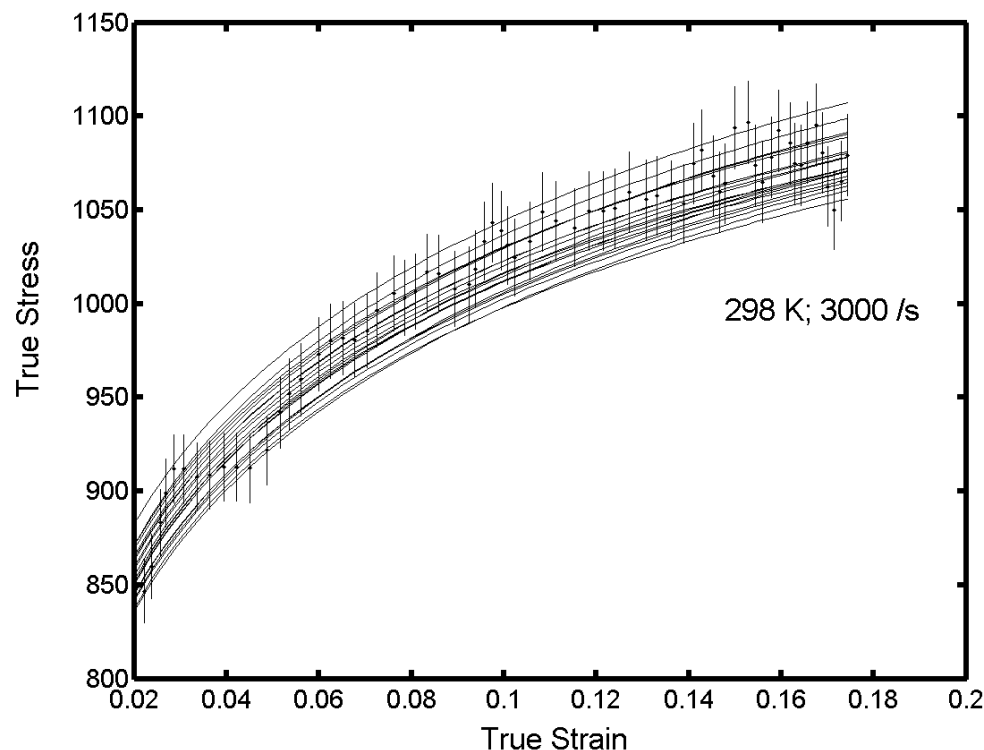
α_1	103 ± 33
α_2	954 ± 63
α_3	0.00408 ± 0.00059
α_4	0.000117 ± 0.000029
α_5	996 ± 22
α_6	0.247 ± 0.021

	α_1	α_2	α_3	α_4	α_5	α_6
α_1	1	-0.083	0.372	0.207	-0.488	0.267
α_2	-0.083	1	0.344	0.311	0.082	0.130
α_3	0.372	0.344	1	0.802	0.453	-0.621
α_4	0.207	0.311	0.802	1	0.271	-0.466
α_5	-0.488	0.082	0.453	0.271	1	-0.860
α_6	0.267	0.130	-0.621	-0.466	-0.860	1

Correlation matrix

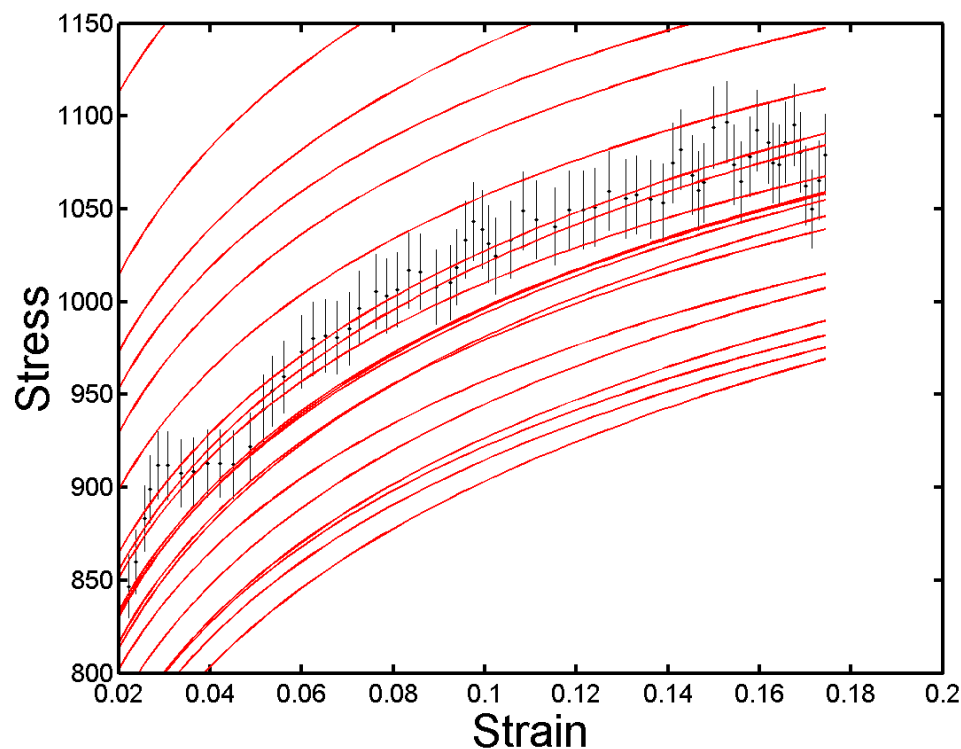
Monte Carlo sampling from posterior

- Use Monte Carlo technique to draw random ZA parameter vectors from their uncertainty distribution
- Plot corresponding curves for room temperature, high strain rate and compare to measurements
- Conclude that parameters and their uncertainties inferred from last slide plausibly represent the data for target conditions



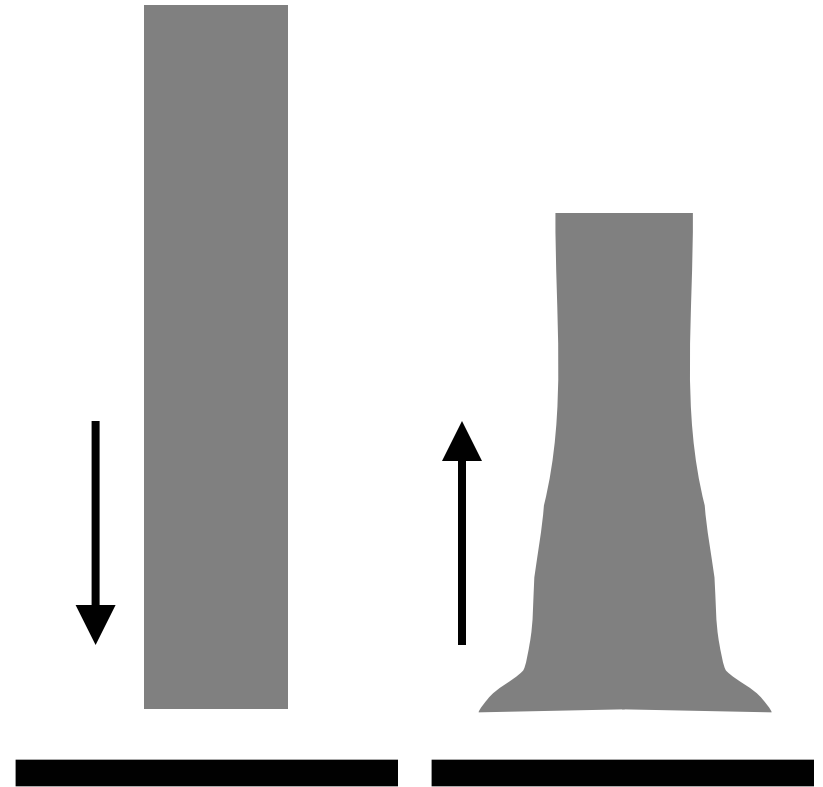
Monte Carlo sampling from posterior

- Plot shows what happens when one uses just the diagonal elements of covariance matrix; that is, **correlations** between parameters are **ignored**
- Conclude that correlations must be included to properly characterize uncertainties



Taylor impact test

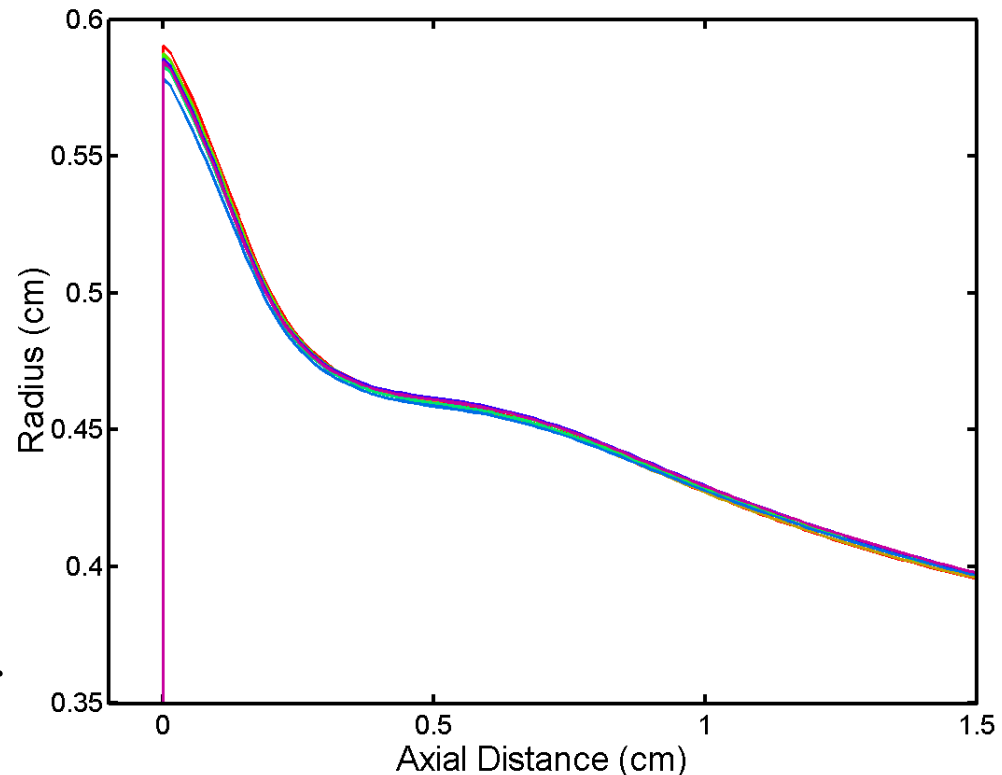
- Propel cylinder into rigid plate
- Measure profile of deformed cylinder
- Deformation depends on
 - ▶ cylinder dimensions
 - ▶ impact velocity
 - ▶ plastic flow behavior of material at high strain rate
- Useful for
 - ▶ determining parameters in material-flow model
 - ▶ validating simulation code (including material model)



Monte Carlo example - Taylor test

- Use MC technique to propagate uncertainties through deterministic simulation code
 - ▶ draw values of six parameters from correlated Gaussian pdf
 - ▶ run CASH code for each set of parameters
- Figure shows range of variation in predicted cylinder shape implied by uncertainties in ZA parameter from previous fit

Predictions made with hydrocode CASH

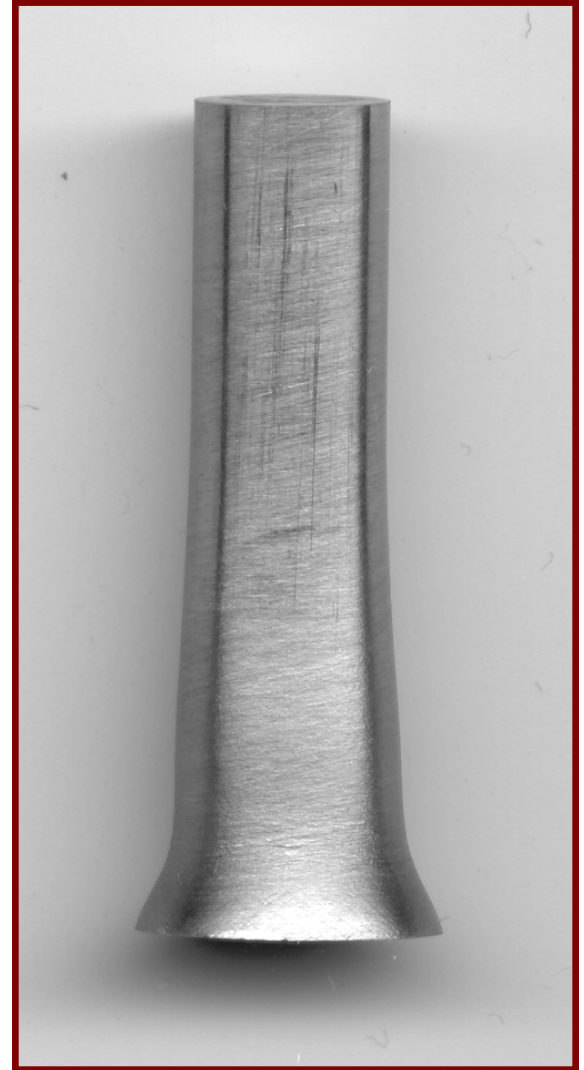


High-strength steel HSLA 100
246 m/s impact velocity

†CASH code from Tom Dey, X-7

Taylor test experiment

- Taylor impact test specimen
 - ▶ high-strength steel HSLA 100
 - ▶ impact velocity = 245.7 m/s
 - ▶ dimensions, final/initial
 - length 31.84 mm / 38 mm
 - diameter 12.00 mm / 7.59 mm



Future work

- Demonstrate how model inference can be done through analysis of Taylor experiments using a simulation code
- Hierarchical Bayesian modeling
 - ▶ use distributions for unknown parameters, e.g., priors on variance in systematic errors (as opposed to specific, fixed values)
 - ▶ infer all parameters and their uncertainties from data & priors
 - ▶ provides more flexibility in modeling uncertainties
- Develop statistical approach to minimize uncertainty for targeted range of variables
- Application to other materials and strength models

Bibliography

- ▶ *Data Analysis: A Bayesian Tutorial*, D. S. Sivia (Clarendon, 1996); excellent introduction to Bayesian analysis for physicists & engineers
- ▶ *Data Reduction and Error Analysis for the Physical Sciences*, P. R. Bevington and D. K. Robinson (Boston, WCB/McGraw-Hill, 1992); good summary of conventional data analysis for physical scientists and engineers
- ▶ “A framework for assessing confidence in simulation codes,” K. M. Hanson and F. M. Hemez, *Experimental Techniques* **25**, pp. 50-55 (2001); application of uncertainty quantification to simulation codes with Taylor test as example
- ▶ “A framework for assessing uncertainties in simulation predictions,” K. M. Hanson, *Physica D* **133**, pp. 179-188 (2000); integrated approach to determining uncertainties in physics modules and their effect on predictions

Last two papers available at <http://www.lanl.gov/home/kmh/>