Optimized alignment of specular specimens for TMARS

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Introduction

Target Material Angle Resolved Scatterometer (TMARS)

- TMARS is a highly resolved 6 DOF laser scatterometer
- Capable of testing specimens up to 136kg (300lbs)
- Specimen position is controlled with 3 linear actuators and 3 rotational actuators
- During testing, the source stays stationary while the specimen and sensor can independently rotate about a common axis

TMARS is used to perform Theta-2Theta scans

- The figure below shows a top-down view of the test set up. Only 4 of the actuators are used during testing; 3 for the specimen and 1 for the sensor
- During data acquisition, the specimen is rotated through a range of angles while the sensor is rotated by twice that range. Ideally, this allows the sensor to "track" the specular reflection from the specimen

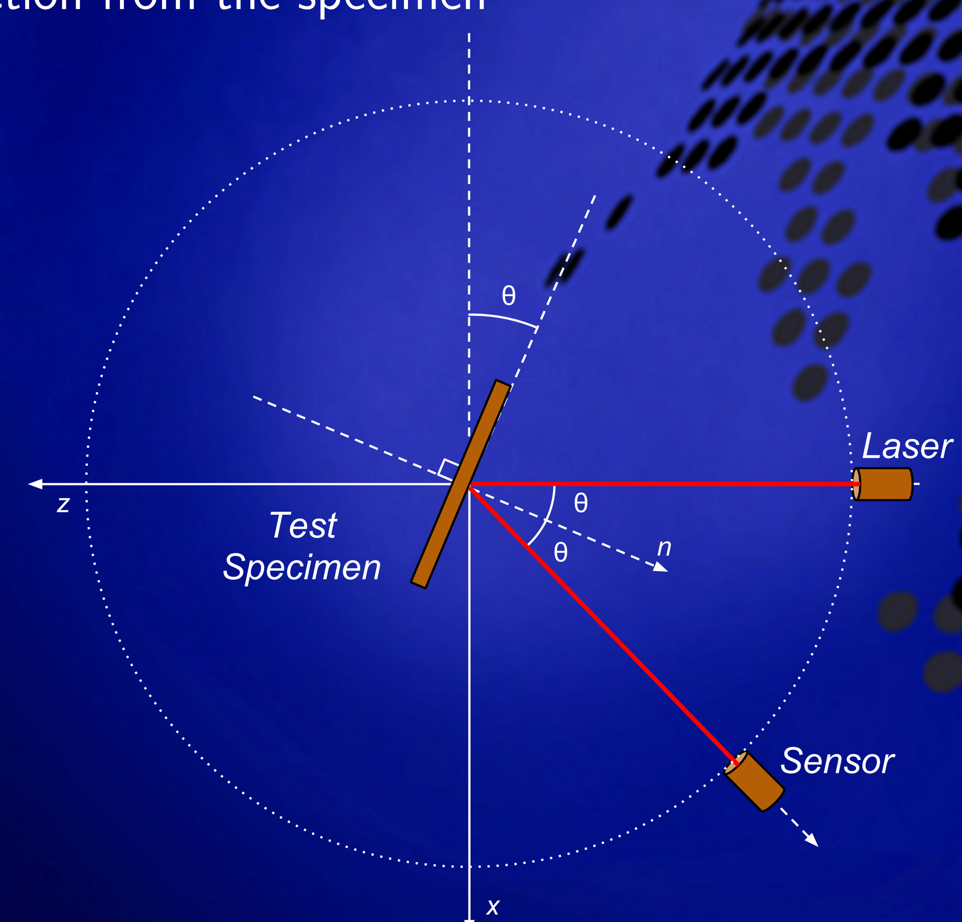


Figure: Test set-up

The specimen is mounted on TMARS by a human operator

- During set-up the actuators are moved so that the axis of rotation lines up with the surface of the specimen
- The set-up process is subject to error as depicted in the figure below
- Small errors in positioning are magnified at a distance and lead to large errors at the sensor. These errors become apparent during a Theta-2Theta scan

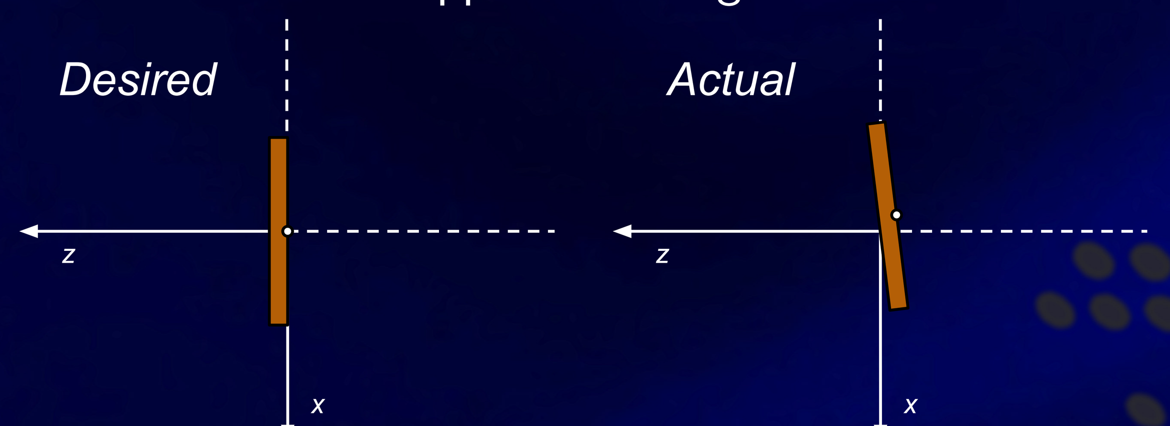


Figure: Positioning error

Objective

- Design an algorithmic method to optimize the final positioning of the specimen
- Method should require no additional hardware
- Should be automated in order to remove human error

Approach

Modeling and Simulation

- A kinematic model was developed to simulate and control the geometric relations between the source, specimen, and sensor. The dependent relations of the coordinate frames are described in the flowchart below.
- The model is used to determine the distance between the reflected source beam and the sensor. The intensity at the sensor is then calculated with a Gaussian beam assumption
- The model is a function of:

  Joint parameters – $(\theta_d, \theta_c, X_c, \& Z_c)$ & Specimen parameters – $(\theta_s, X_s, \& Z_s)$

Sensor (θ_d) ← Base frame → Rotational offset (θ_c) → Specimen mount $(X_c \& Z_c)$ → Specimen surface $(\theta_s, Z_s, \& X_s)$

Figure: Kinematic flowchart

Optimization

- Several observations are simulated by perturbing the initial state. In a real world system this data would come from the actual sensor readings
- During optimization, it is assumed that the specimen parameters are not known. The optimization algorithm then seeks the model which most closely matches the observed data by maximizing the error function

Observation Simulation

Assume initial values for $(\theta_s, X_s, \& Z_s)$
↓
Simulate test set-up by operator by placing specimen with some Gaussian noise
↓
For each observation, generate a Gaussian perturbation about the initial state
↓
For each perturbation, simulate a Theta-2Theta scan
↓
Maximize the error function, E, with respect to $\theta_s, X_s, \& Z_s$

Figure: Optimization procedure

The error function contains a global maxima where there is no difference between the observed intensities and the intensities predicted by the model:

$$E = e^{-\sum_{i=1}^{N} mean|I_{observed} - I_{model}|}$$

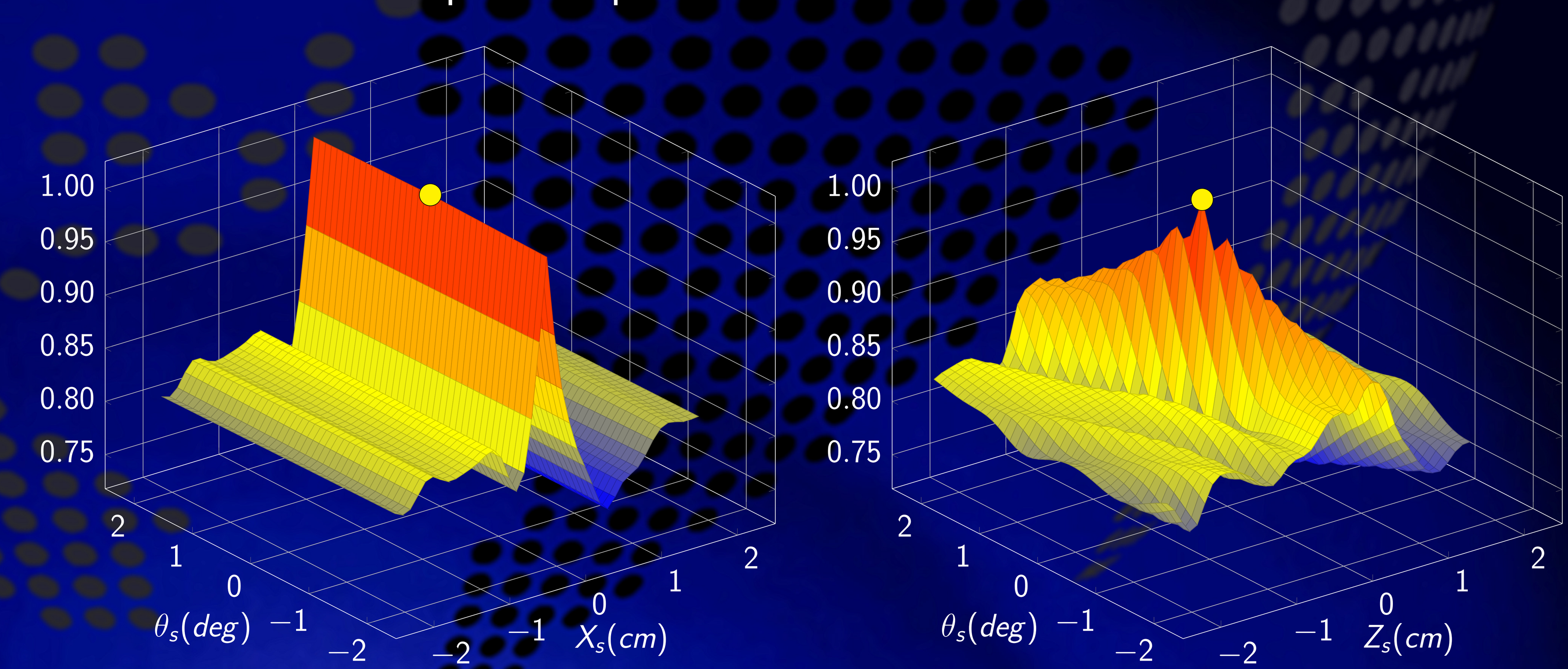
Results to Date

Creating model and visualizing simulated data

- Matlab code has been written to simulate the kinematic model and the resulting Theta-2Theta scan. Also, a script has been written to simulate gathering real world observations
- A Matlab GUI has been developed to allow easy manipulation and visualization of all aspects of the simulation

Exploration of the error function space

- Figures below show the error function plotted against $\theta_s, X_s, \& Z_s$. The yellow dot indicates the actual specimen parameters



(a) S_x vs. S_θ (b) S_z vs. S_θ

Figure: Plot of $E(\theta_s, X_s, Z_s)$

- The ridge in figure (a) shows that when Z_s and θ_s are correct, X_s can move and give an equally valid solution. The error function will need to be modified in order to penalize movement

Conclusion/Future Work

- The error function seems to be well behaved. This indicates that a robust optimization procedure is possible.
- Plotting and visualization have revealed that the current error function has many valid solutions. In order to arrive at one optimal solution a penalty term must be designed and added
- Future simulation work includes: adding real world affects such as noisy data and the signal integration created by the aperture
- The end goal is to implement the algorithm into the actual hardware and software of TMARS