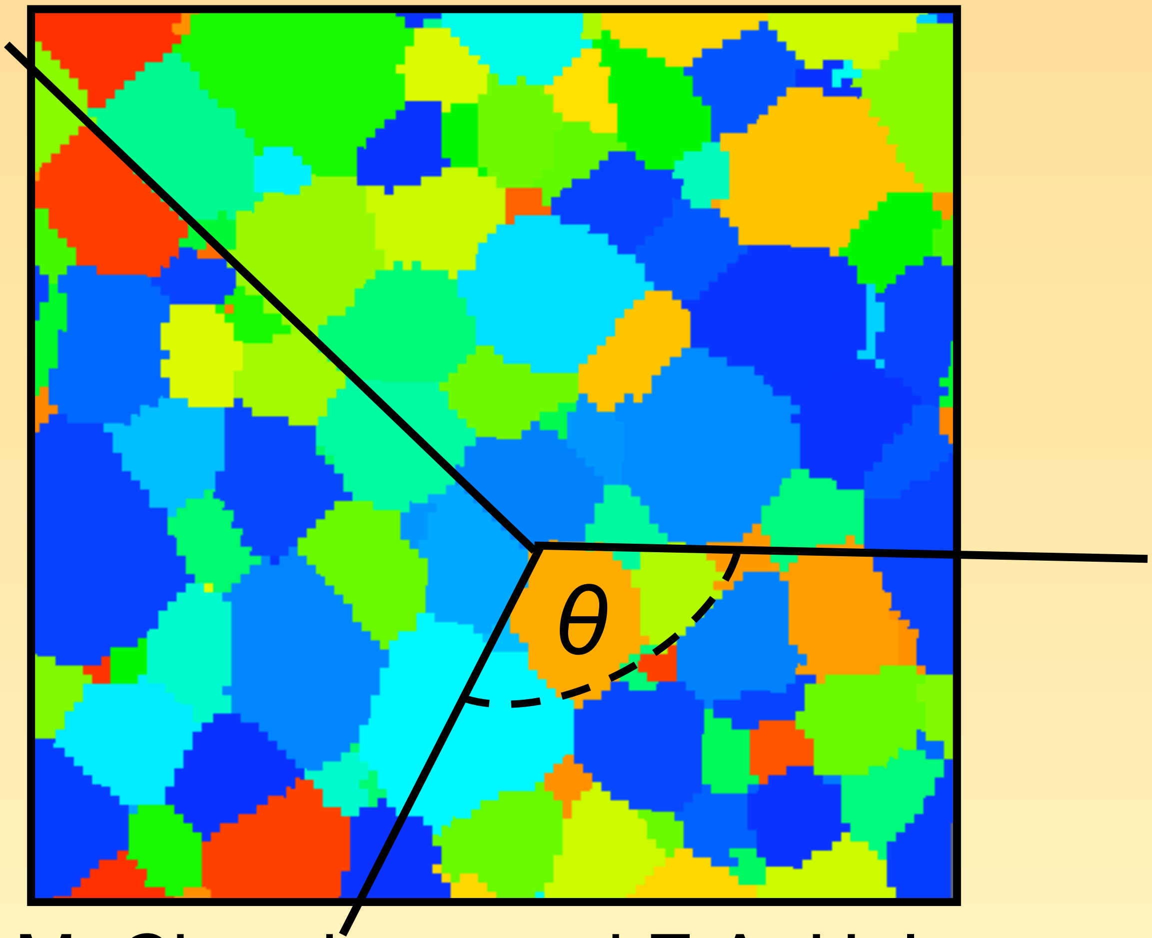
SAND2010-0913C

# Calculation of Grain Boundary Angles in 3D Digitized Microstructures

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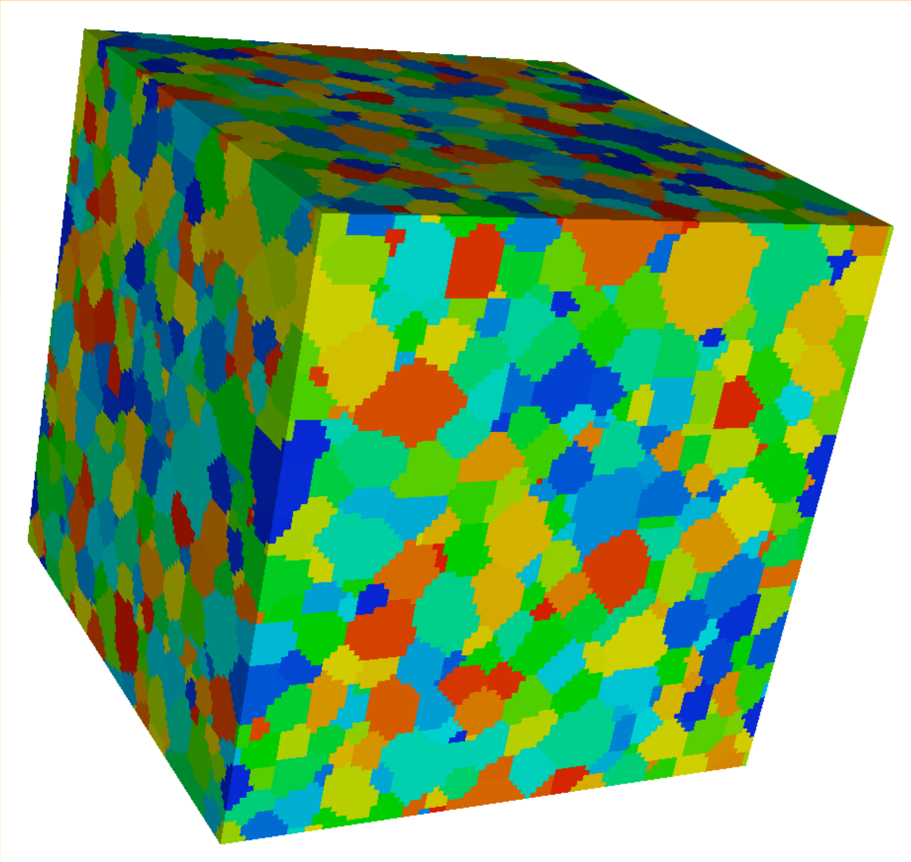
# Introduction:  Why?

- Grain boundary angles control:
  - microstructure morphology
  - grain shape
- Angles arise from balance of surface tensions
- Isotropic energies:  angles = 120°
- Varying energies:
  - Angles deviate
  - Quad junctions

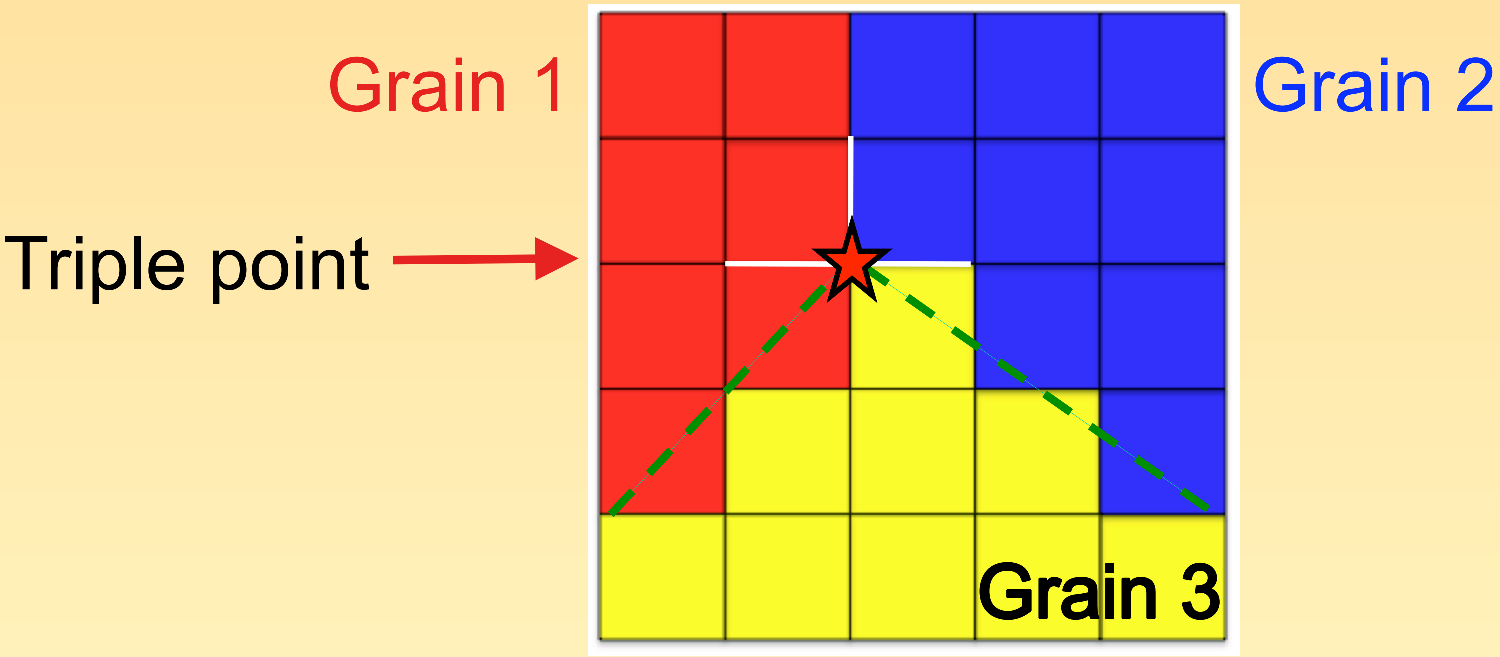


# Introduction: Why not?

- Previous representations were analog, now digital
  - Protractor vs. computer
  - Explicit vs. implicit boundaries
- Tangents are not uniquely defined
- Always looking at 2D section of 3D structure – what is the correct distribution?

# Method:  Desired Results

We want angles between tangents to grain boundaries in discretized microstructures



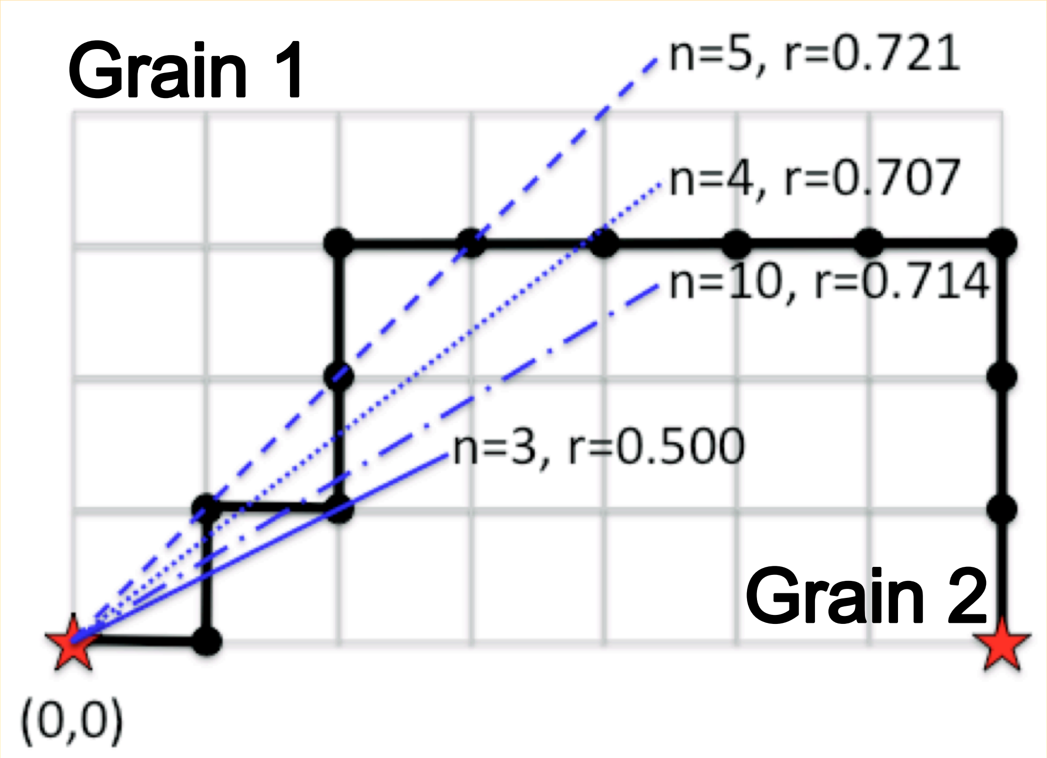

What are the tangents?

Extreme case:  One segment away:  90° or 180°

Better solution:  Curve fitting

# Method: A Series of Linear Fits

Starting vertex




Ending vertex

1) Find all triple/quad points (vertices)
2) For a given vertex, map out all emanating boundaries
3) Find best linear fits to each of those boundaries
4) Find angles between those linear fits

# Fitting Method: Linear Regression

- Constrain line to start at origin (i.e. vertex)

$$y = ax$$

- Set $\chi^2$ =0 for the number of points to be fit (i.e. number of points along the boundary)

$$\chi^2 = \sum_{i=1}^{n} (y_i - ax_i)^2$$

$$a = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$$

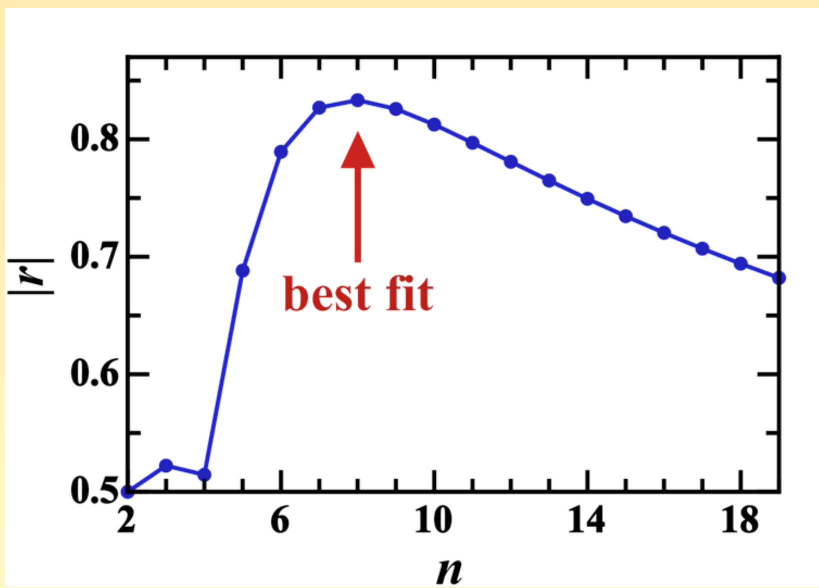
- Gives a different line for each n. Which is best?

# Best Line: Pearson's Correlation Coefficient

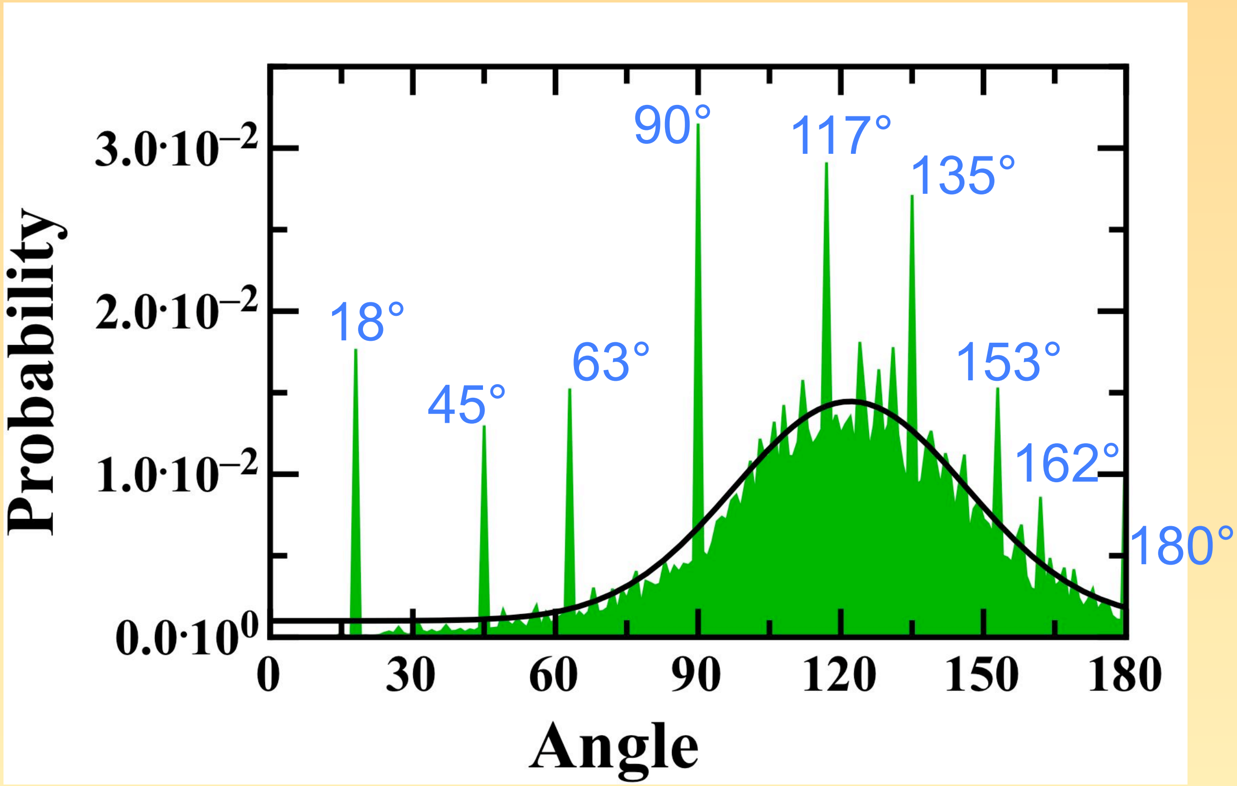
- Divide the covariance of two variables by their standard deviation

$$r = \frac{\mathrm{cov}(x,y)}{\sigma_x \sigma_y} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

- Gives the amount of correlation between two variables (here: how reasonable is a linear fit?)

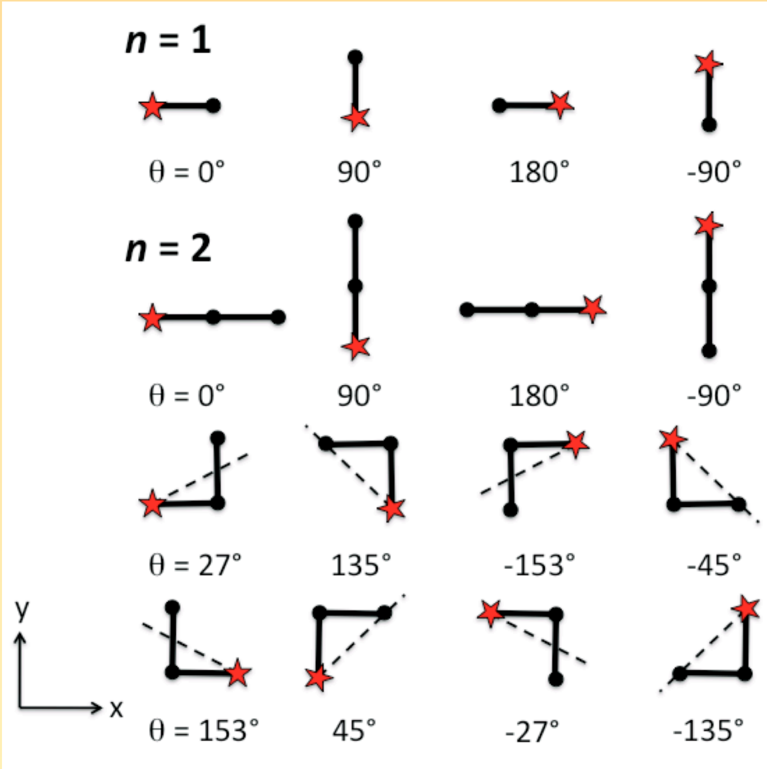


# Results: Example Distribution



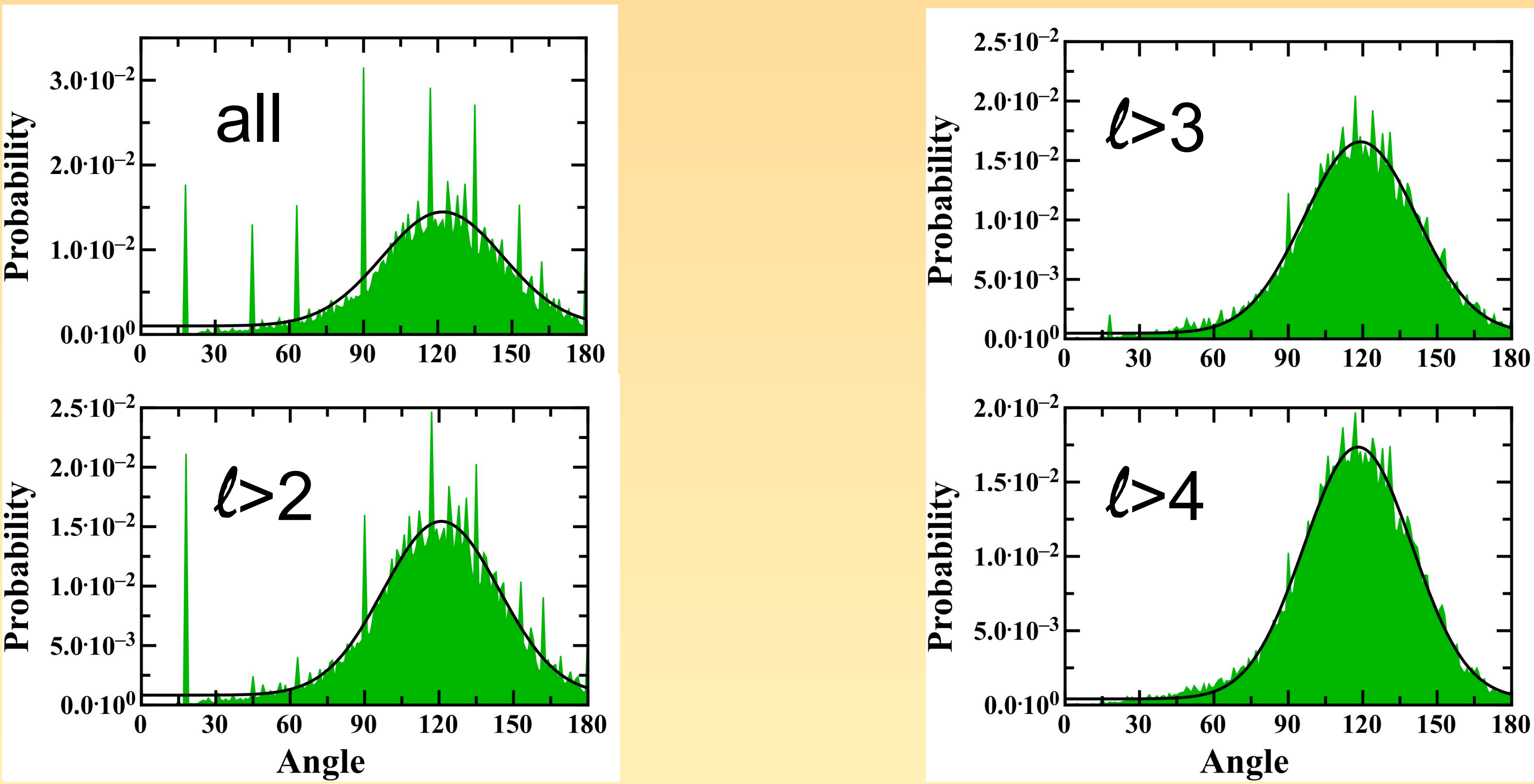

- 3D MC Potts model, $150^3$, T=1.5, 100 timesteps
- Calculation for series of 2D slices separated by grain radius
- Averaged over all three dimensions
- Fits well to Gaussian centered at 120°, except for peaks

# Taxonomy of Short Segments



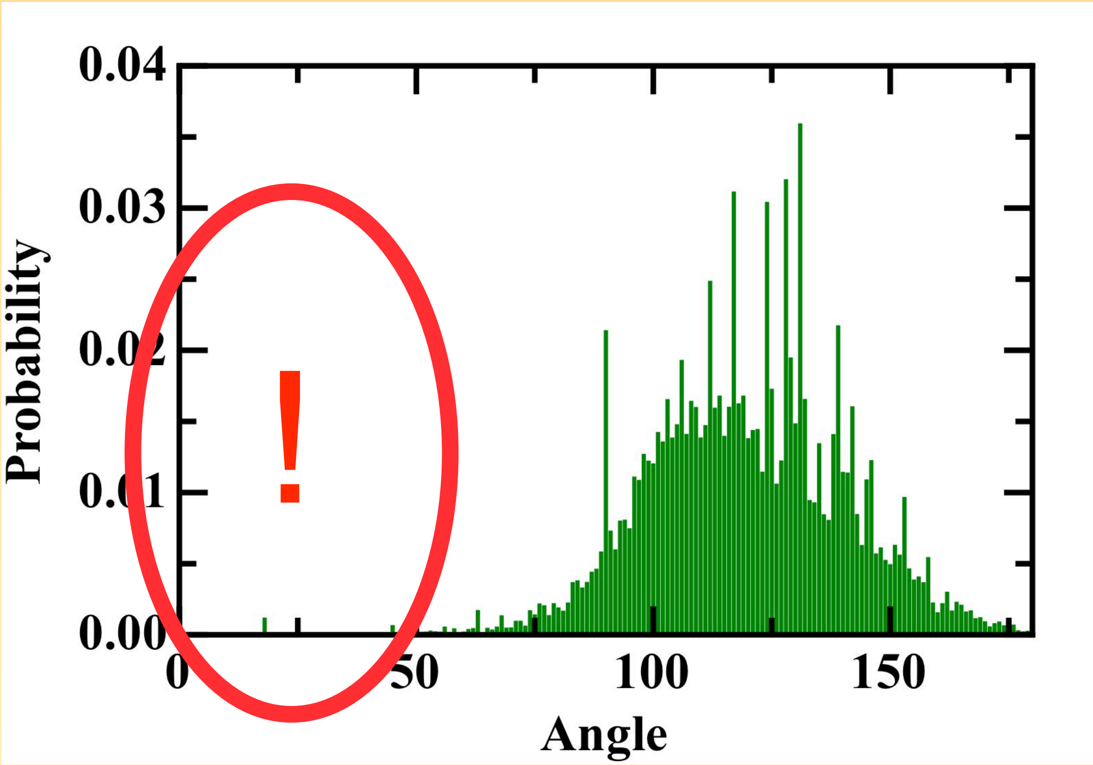

- All fits to boundaries of length 1 and 2
- Angles come from *differences* (i.e. 45° – 27° = 18°)
- Prove this by restricting the length of boundaries in analysis

# Removing the Short Boundaries



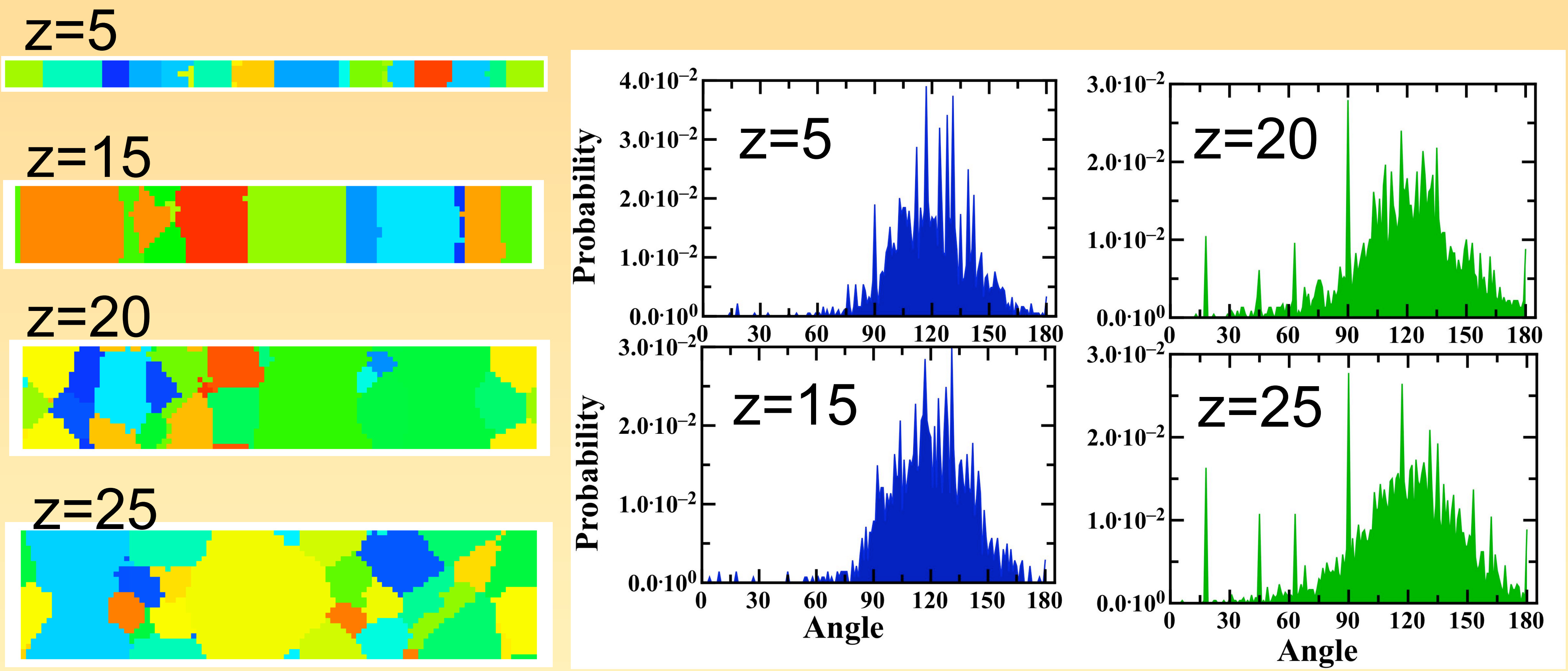

- Short boundaries unavoidable in 2D slices of 3D microstructures
  - Shrinking and/or disappearing grains
  - Most slices not on equator

# Short Boundaries are a 3D Effect



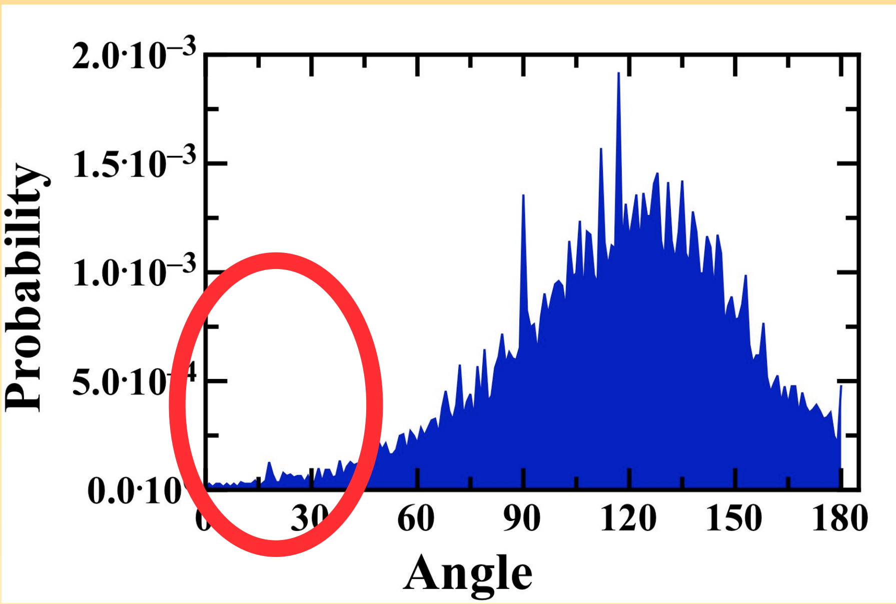

- 2D calculation, $1000^2$, T=1.5, 100 timesteps
- Gaussian, peaked near 120°, skewed to high angles
- Low angle peaks are gone. Can we exploit this?

# Exploitation!

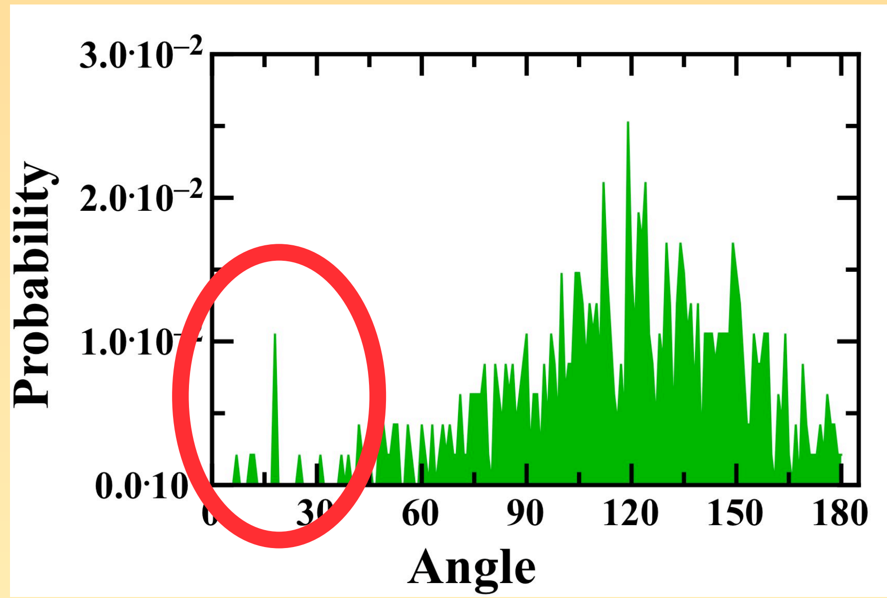



- Increase thickness of film to transition between columnar and equiaxed
- Low angle (18°) peak distinguishes between 2D and 3D

# Experimental Verification



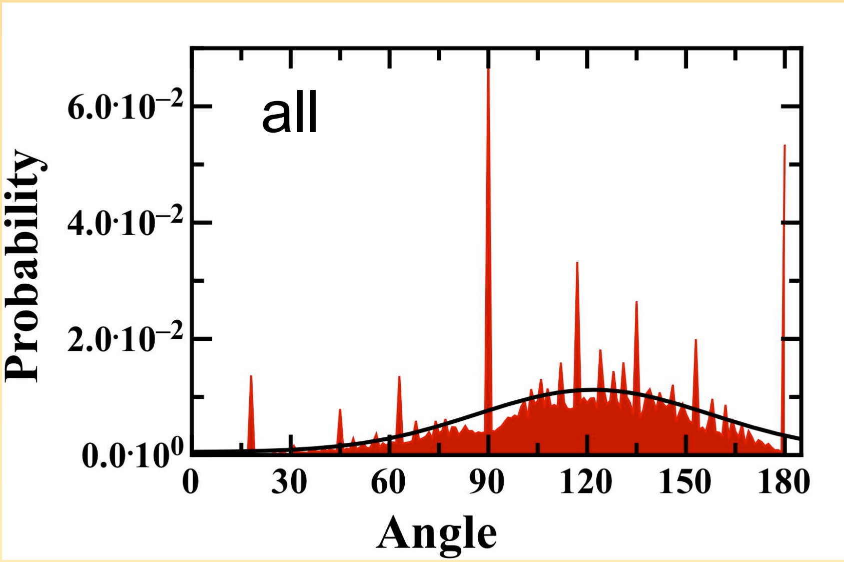

1.7 *μm* columnar Al film
(courtesy K. Barmak and G. Rohrer)

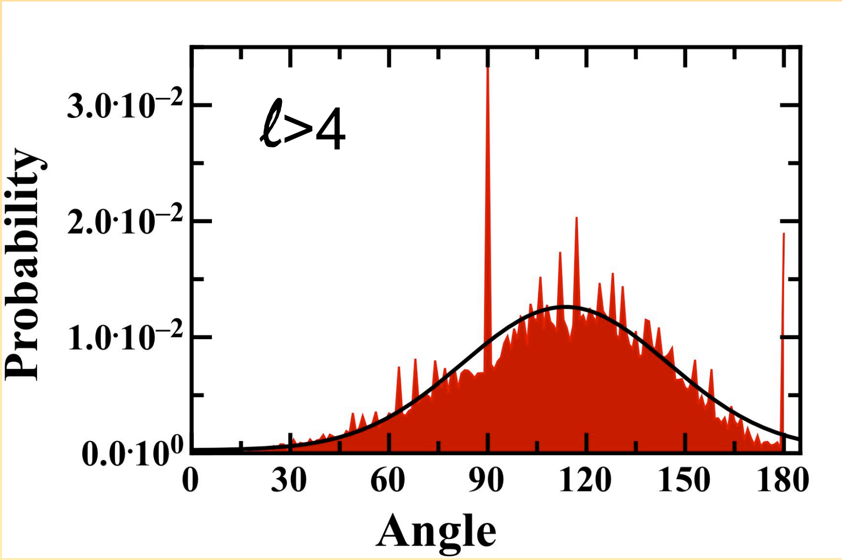



1.6 mm Ni tensile bar
33 *μm* equiaxed grains
twins removed
(courtesy L. Brewer)

- Works for experimental films, too
- Non-destructive technique

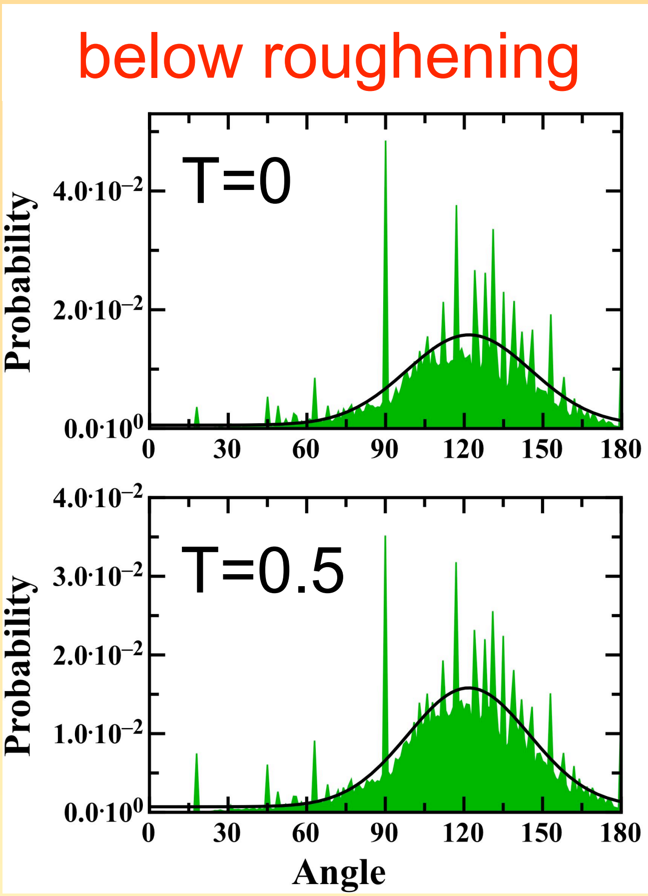
# How Much Would You Pay? Don't Answer Yet!

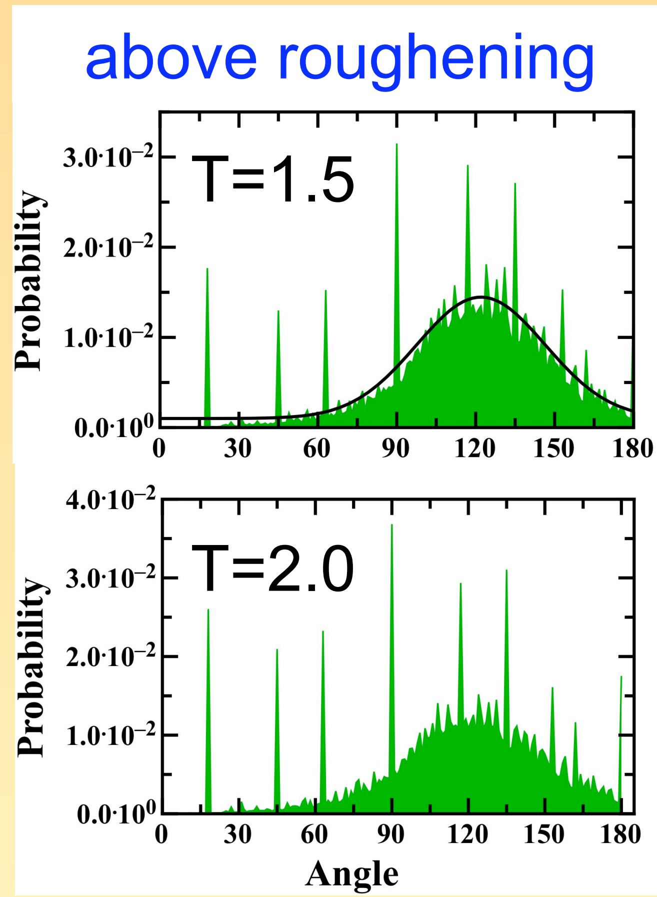



- Indicates issues with Voronoi tesselation
- Same system size as Potts simulations ($150^3$), topologically similar
- Massive peaks at 90, 180 – lattice effects

# Another Use: Simulation Temperature




- Can help determine appropriate simulation temperature
  - Below roughening, faceting gives peaks at 90° and 180°
  - Above roughening, peaks are temperature independent

# Conclusions

- Robust method for determining triple junction angles
- Many uses:
  - Validation of simulation parameters/methods
    - Temperature
    - Voronoi tesselation vs. Potts model
    - Roughening
  - Dimensionality of sample
    - Columnar vs. Equiaxed grains
    - Suitable for simulations and experiments
    - Non-destructive surface probe technique
    - Further analysis may lead to degree of columnarity (peak ratios, etc.)