Modeling of Processing Path of Ti During Mechanical Deformation

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Outline

- Background
- Processing Path Model
  - Processing path function
  - Streamline
- Application in Titanium
  - hexagonal (α phase)
  - cubic (β phase)
- Conclusion

Representation of Texture

ODF is defined as

$$f(g,\eta) = \sum_{l=0}^{\infty} \sum_{m=0}^{M(l)} \sum_{n=0}^{N(l)} F_l^{mn}(\eta) \ddot{T}_l^{mn}(g)$$

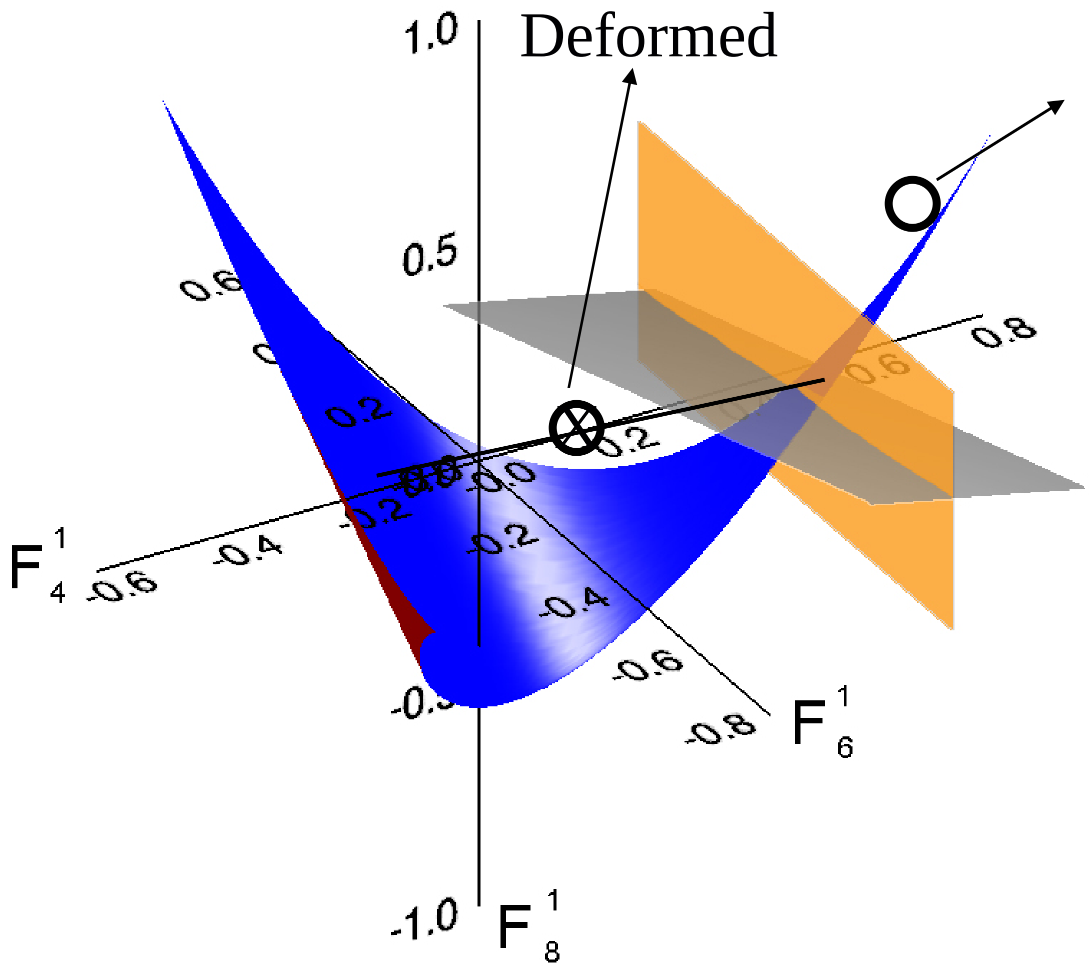
Representation of texture: $\{F_l^{\mu\nu}\}$

Representation of properties:

$$\bar{e}_l^{\mu\nu} = \frac{1}{2l+1} \sum_{\lambda=1}^{M(l)} e_l^{\mu\lambda} F_l^{\lambda\nu} \qquad 0 \le l \le r$$

r: order of property

Microstructure Sensitive Design
Processing Solutions

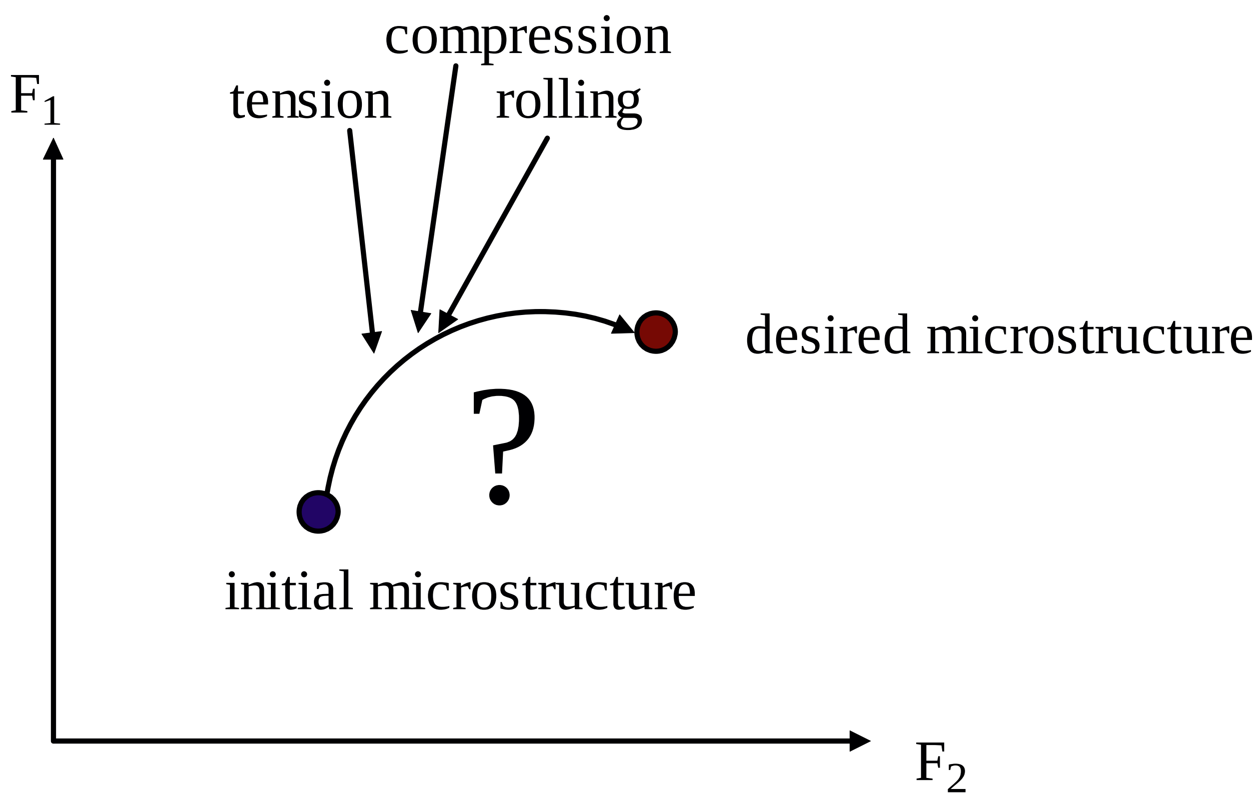


Deformed and Annealed

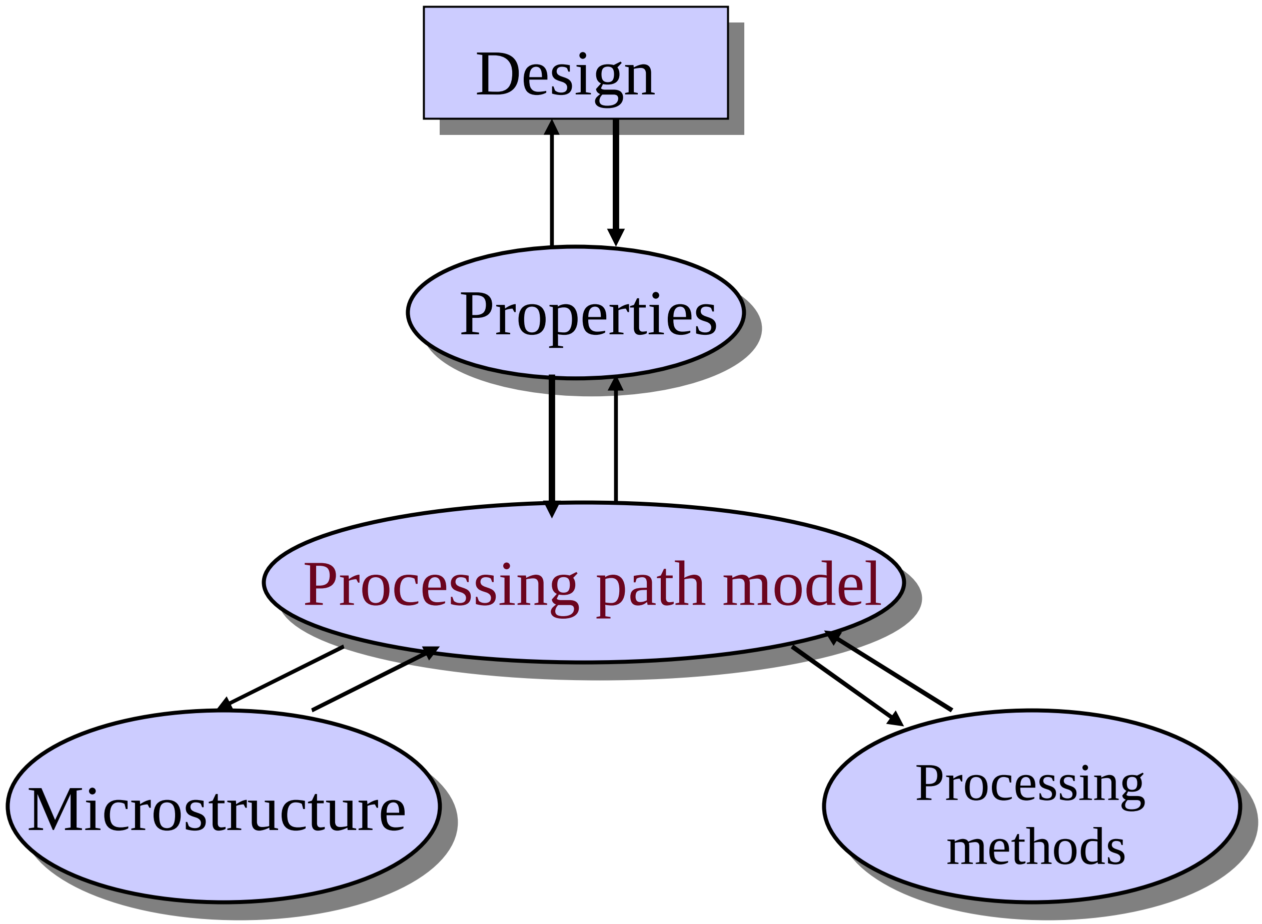
Linear combination
provides
desired properties

Question:

How to find the processing path from initial microstructure of the raw material to final microstructure with desired properties?



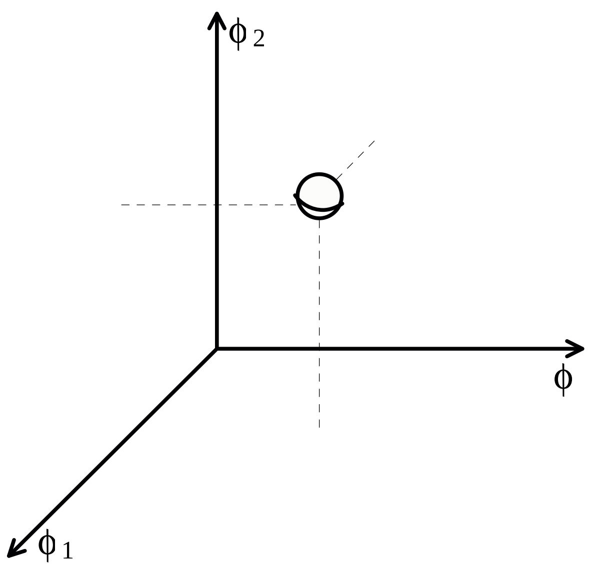
Microstructure Sensitive Design



Principle of Conservation in Orientation Space

In the orientation space $dv = d\varphi_1 d\varphi d\varphi_2$

while $dg = \frac{1}{8\pi^2} \sin\varphi d\varphi_1 d\varphi d\varphi_2$



The normalization relation for texture is:

$$\iiint f(g) dg = 1$$

So the density is defined as:

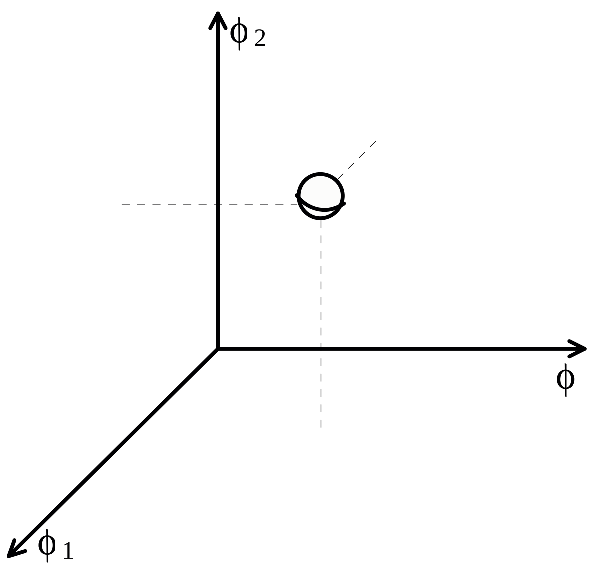
$$\rho = \frac{1}{8\pi^2} f(g) \sin\varphi$$

to satisfy the normalization

$$\iiint \rho dV = 1$$

Quantity of matter moving out of the infinitesimal volume

$R(\varphi_1, \varphi, \varphi_2)$ Rotation field, represent the flow vector of any point (φ_1, φ, φ_2) in this space



flux across the element surface is :

$$\rho R \cdot n d\sigma$$

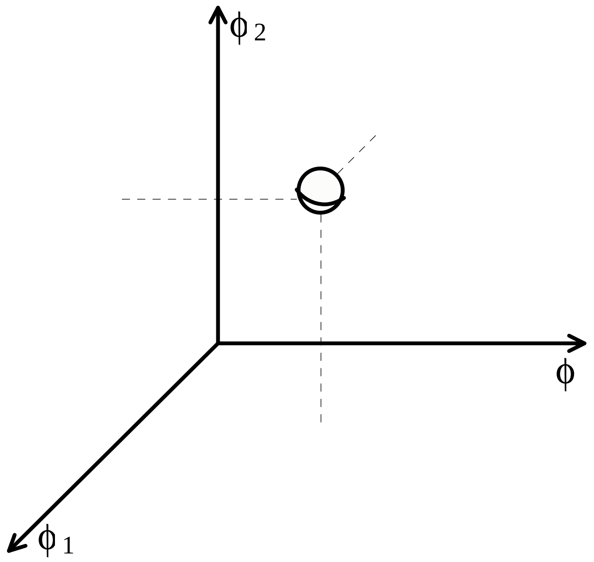
The quantity of matter moving across S is:

$$\oint_S \rho R \cdot n d\sigma = \frac{1}{8\pi^2} \oint_S f(g) \sin\phi R \cdot n d\sigma$$

$$= \frac{1}{8\pi^2} \iiint_V div\{f(g)\sin\phi R\} dV$$

Change of Quantity of matter in the infinitesimal volume

The increase in the quantity of matter in infinitesimal volume *V* in unit time is:

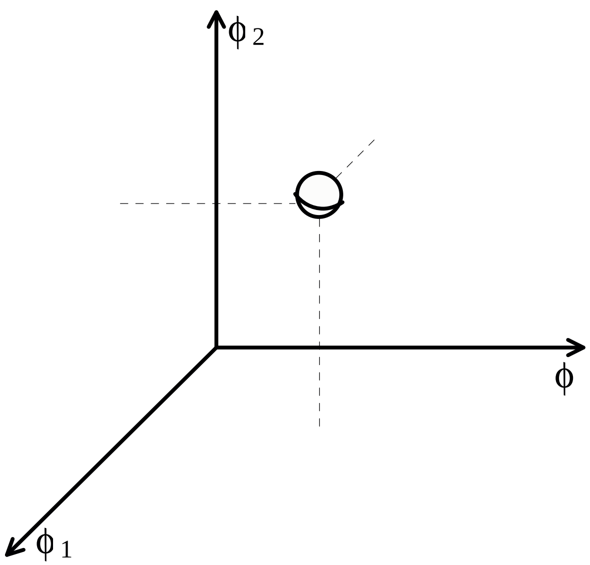


$$\frac{\partial}{\partial t}\iiint_V \rho dV$$

$$= \frac{\partial}{\partial t}\iiint_V f(g)\frac{1}{8\pi^2}\sin\phi dV$$

Principle of Conversion in Orientation Space

According to the conservation principle:



$$\frac{\partial f(g)}{\partial t} + \frac{1}{\sin\phi} div[f(g)\sin\phi R(g)] = 0$$

$$\frac{\partial f(g,\eta)}{\partial t} + div[f(g,\eta)R(g)] + ctg\phi f(g,\eta)R(g) = 0$$

Using the spectral expansion, we have

$$f(g,\eta) = \sum_{l=0}^{\infty}\sum_{m=0}^{M(l)}\sum_{n=0}^{N(l)} F_l^{mn}(\eta)\overset{\therefore}{T}_l^{mn}(g)$$

Substituting into the conservation principle

$$\sum_{lmn}\frac{dF_l^{mn}(\eta)}{d\eta}\overset{\therefore}{T}_l^{mn}(g) + \sum_{\lambda\sigma\rho} F_\lambda^{\sigma\rho}(\eta)\left(div\left(\overset{\therefore}{T}_\lambda^{\sigma\rho}(g)R(g)\right) + ctg\phi\overset{\therefore}{T}_\lambda^{\sigma\rho}(g)R(g)\right) = 0$$

Processing Path Model During Plastic Deformation

$$\sum_{lmn} \frac{dF_l^{mn}(\eta)}{d\eta} \dot{\ddot{T}}_l^{mn}(g) + \sum_{\lambda\sigma\rho} F_\lambda^{\sigma\rho}(\eta)\left(div\left(\dot{\ddot{T}}_\lambda^{\sigma\rho}(g)R(g)\right) + ctg\phi \dot{\ddot{T}}_\lambda^{\sigma\rho}(g)R(g)\right) = 0$$

If we define

$$div\left(\dot{\ddot{T}}_\lambda^{\sigma\rho}(g)R(g)\right) + ctg\phi \dot{\ddot{T}}_\lambda^{\sigma\rho}(g)R(g) = -\sum_{lmn} A_{l\lambda}^{mn\sigma\rho} \dot{\ddot{T}}_l^{mn}(g)$$

The evolution of F is revealed as:

$$\frac{dF_l^{mn}(\eta)}{d\eta} = \sum_{\lambda\sigma\rho} A_{l\lambda}^{mn\sigma\rho} F_\lambda^{\sigma\rho}(\eta)$$

processing path function $$F(\eta) = e^{A\eta} F(\eta_0 = 0)$$

Processing Path: for Ti (cubic)

In cubic-orthotropic system, *l<=4* when elastic properties are studied. This reduces our interesting texture coefficients to F_4^{11}, F_4^{12} and F_4^{13}

$$\frac{dF_4^{11}(\eta)}{d\eta} = \sum_{\lambda=0}^{L_{\max}} \sum_{\sigma=0}^{N(\lambda)} \sum_{\rho=0}^{M(\lambda)} A_{l\lambda}^{mn\sigma\rho} F_\lambda^{\sigma\rho}(\eta)$$

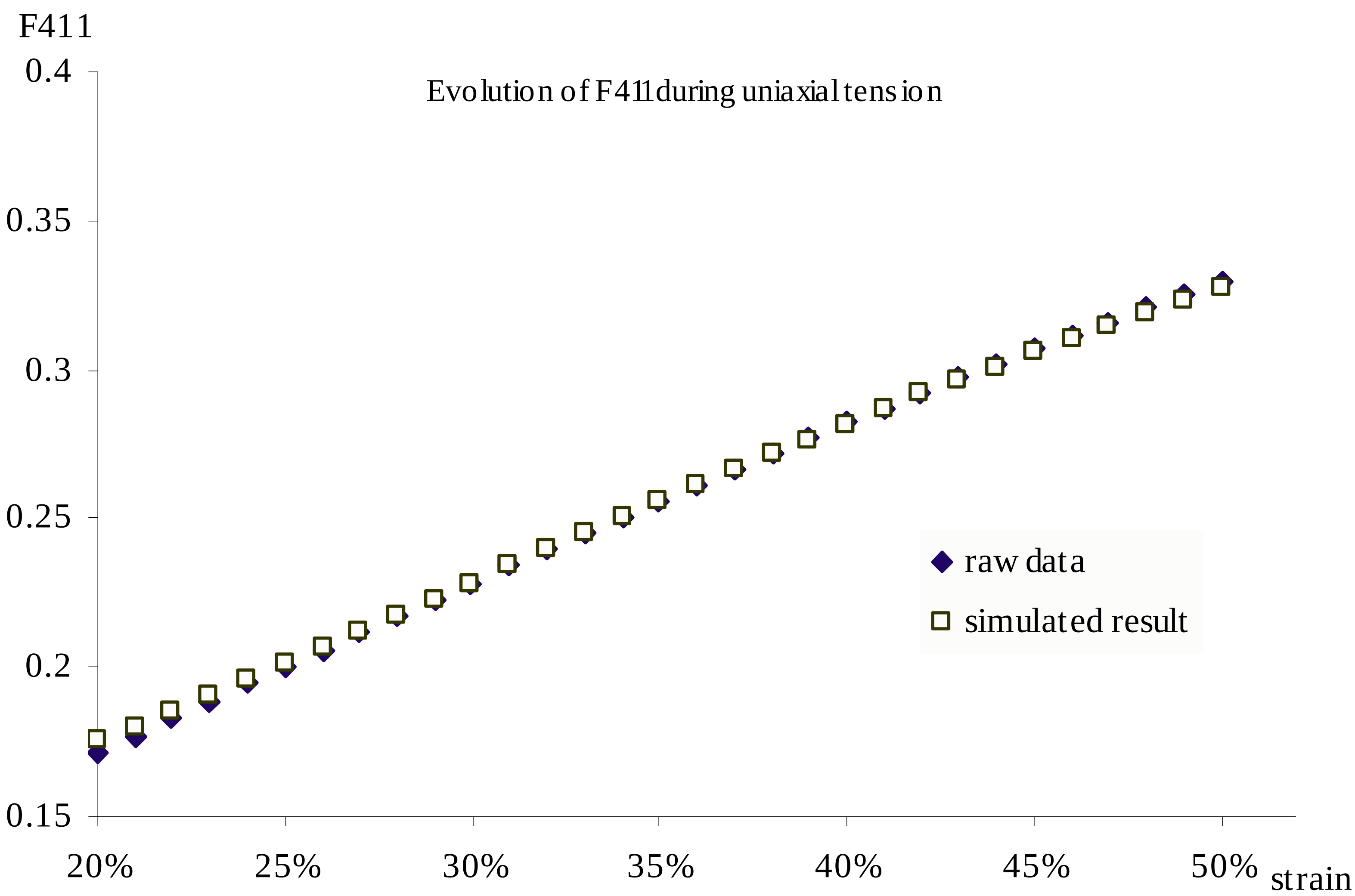
$$= A_{40}^{1111} F_0^{11} + A_{44}^{1111} F_4^{11} + A_{44}^{1112} F_4^{12} + A_{44}^{1113} F_4^{13}$$

$$+ A_{46}^{1111} F_6^{11} + A_{46}^{1112} F_6^{12} + \cdots$$

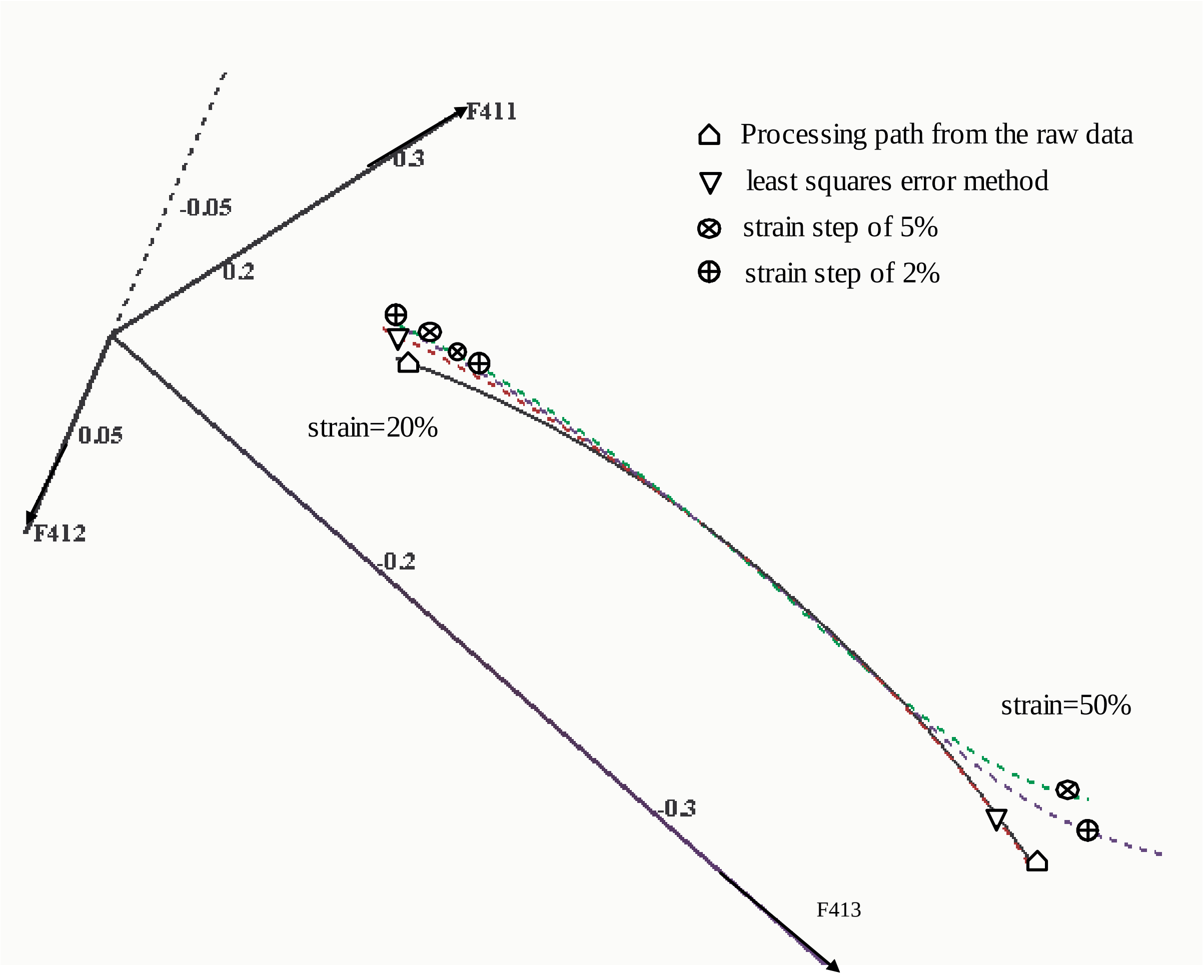
$$\begin{bmatrix} dF_0^{11}/d\eta \\ dF_4^{11}/d\eta \\ dF_4^{12}/d\eta \\ dF_4^{13}/d\eta \end{bmatrix} = \begin{bmatrix} A_{40}^{1111} & A_{44}^{1111} & A_{44}^{1112} & A_{44}^{1113} & \cdots \\ A_{40}^{1211} & A_{44}^{1211} & A_{44}^{1212} & A_{44}^{1213} & \cdots \\ A_{40}^{1311} & A_{44}^{1311} & A_{44}^{1312} & A_{44}^{1313} & \cdots \\ A_{40}^{1411} & A_{44}^{1411} & A_{44}^{1412} & A_{44}^{1413} & \cdots \end{bmatrix} \begin{bmatrix} F_0^{11} \\ F_4^{11} \\ F_4^{12} \\ F_4^{13} \\ \vdots \end{bmatrix}$$

$$F(\eta) = e^{A\eta} F(\eta_0 = 0)$$

Processing Path: Simulation Results

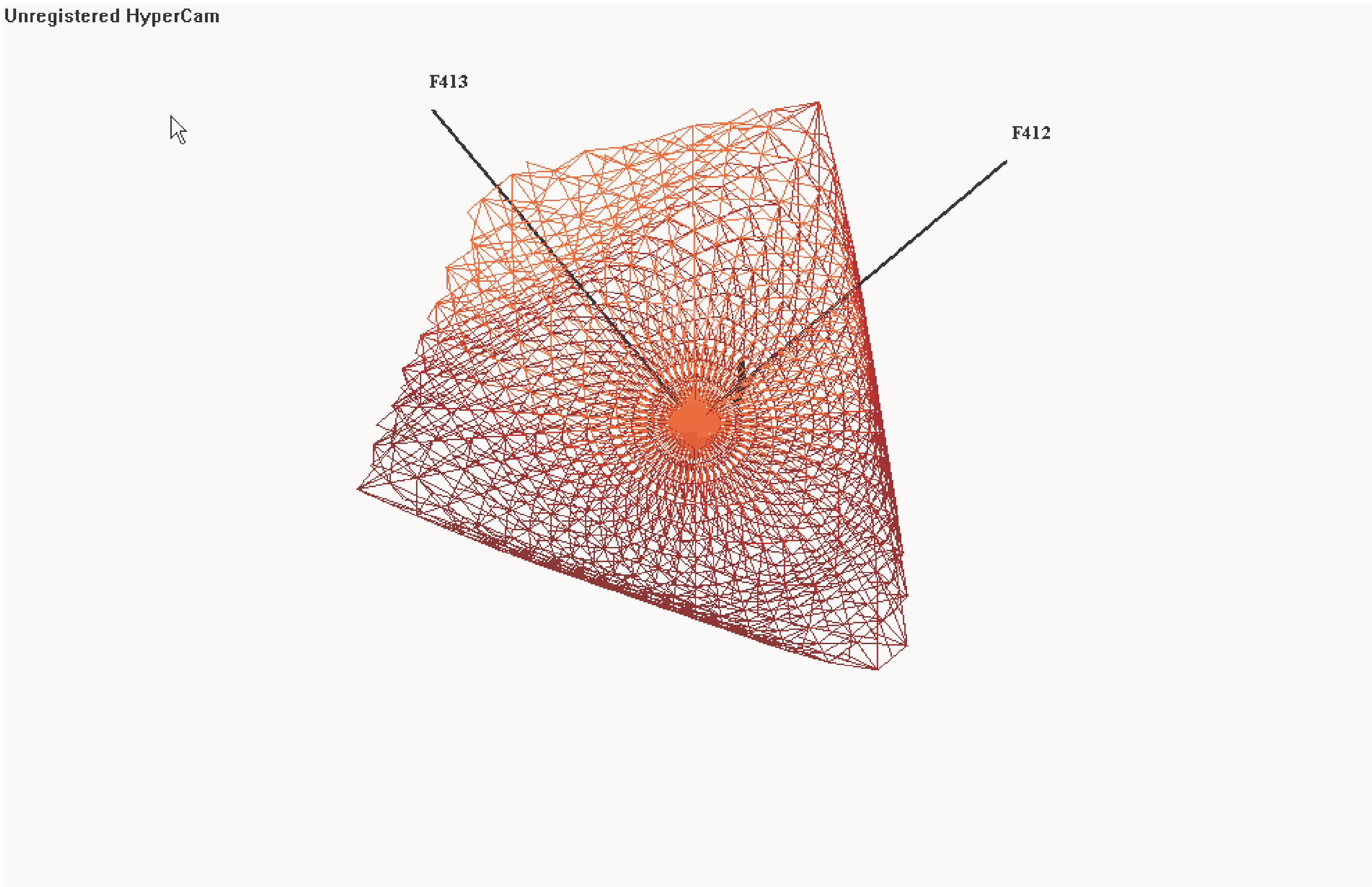


Processing Path



The black solid processing path from raw data is indistinguishable from the red dash processing paths simulated using least squares error method. The green dash processing path simulated by strain step as 5% deviates a little from the processing path of raw data. The blue dash processing path simulated by strain step as 2% deviates more.

Processing Path



Improvement of Simulation Performance by increasing the order of A

$$\frac{dF_4^{11}(\eta)}{d\eta} = \sum_{\lambda=0}^{L_{\max}} \sum_{\sigma=0}^{N(\lambda)} \sum_{\rho=0}^{M(\lambda)} A_{l\lambda}^{mn\sigma\rho} F_\lambda^{\sigma\rho}(\eta)$$

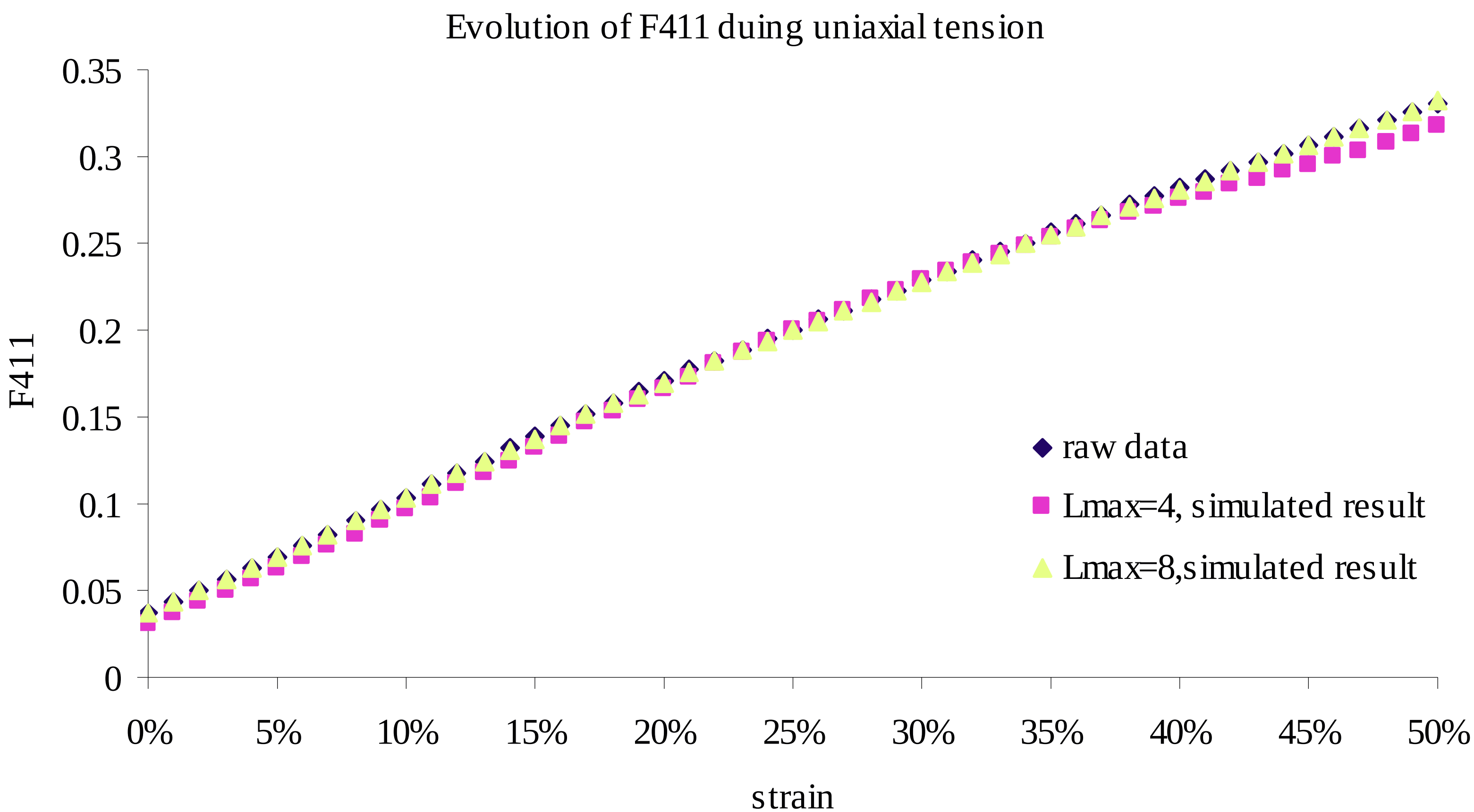
$L_{max} = 4 \rightarrow 8.$

$$\frac{dF_4^{11}(\eta)}{d\eta} = A_{40}^{1111} F_0^{11} + A_{44}^{1111} F_4^{11} + A_{44}^{1112} F_4^{12} + A_{44}^{1113} F_4^{13} + \cdots$$

$$= A_{40}^{1111} F_0^{11} + A_{44}^{1111} F_4^{11} + A_{44}^{1112} F_4^{12} + A_{44}^{1113} F_4^{13}$$

$$+ A_{46}^{1111} F_6^{11} + A_{46}^{1112} F_6^{12} + A_{46}^{1113} F_6^{13} + \ldots + A_{48}^{1115} F_8^{15}$$

Improvement of Simulation Performance by increasing the order of *A*



Increasing the order of texture evolution matrix *A* will improve the performance of simulation.

Streamline

Processing Path Function: $F(\eta) = e^{A\eta} F(\eta_0 = 0)$

If texture evolution matrix A is decomposed into:

$$A = PLP^{-1}$$

$$L = \begin{bmatrix} a_1 & & & \\ & a_2 & & \\ & & \ddots & \\ & & & a_n \end{bmatrix} \qquad P = \begin{bmatrix} \vec{a}_1 & \vec{a}_2 & \cdots & \vec{a}_n \end{bmatrix}$$

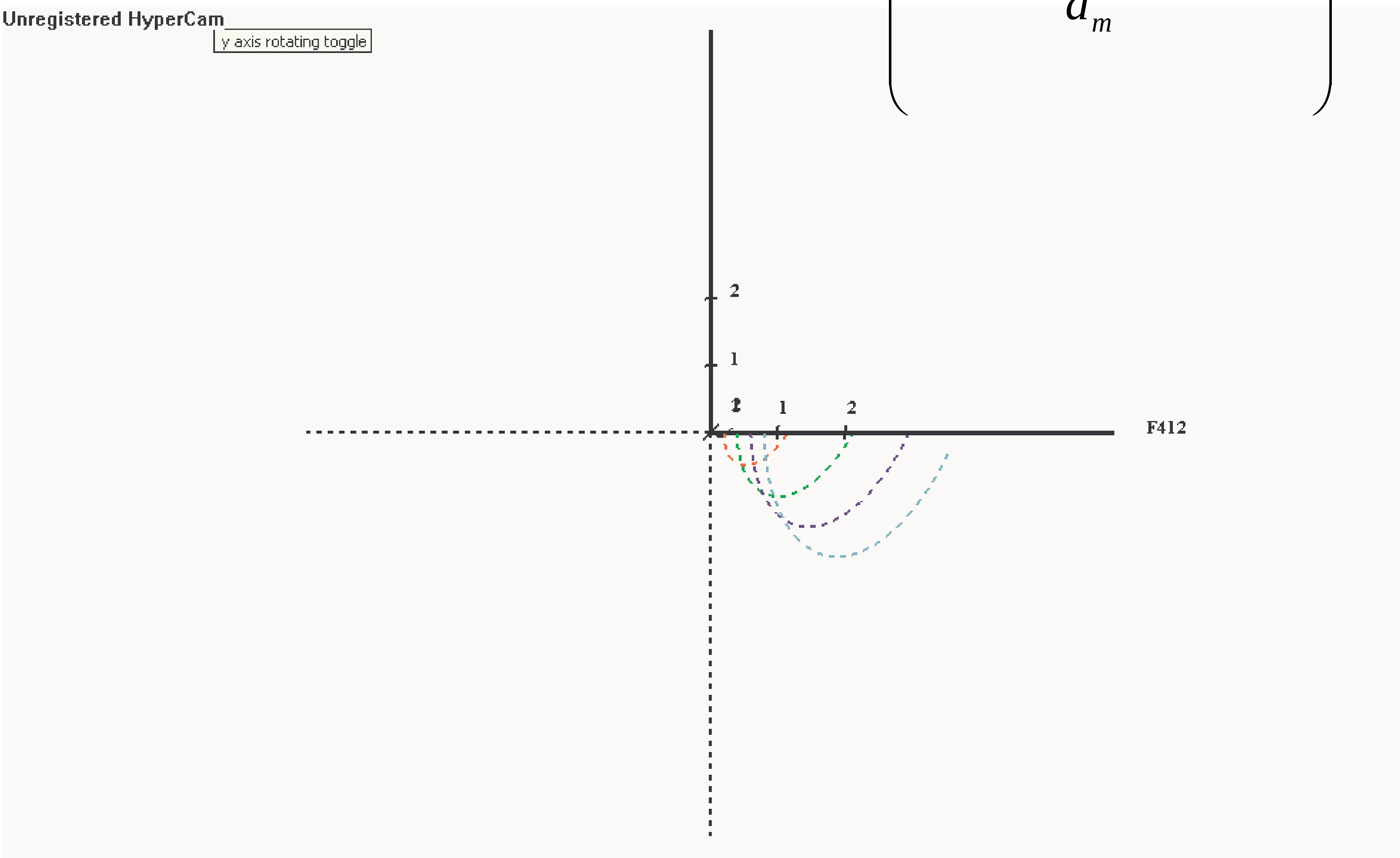
After a series of mathematical derivation, streamline is obtained:

$$\eta = \frac{\ln\left(\dfrac{P^{-1}F(\eta)\cdot e^{m}}{P^{-1}F(\eta_0 = 0)\cdot e^{m}}\right)}{a_m}$$

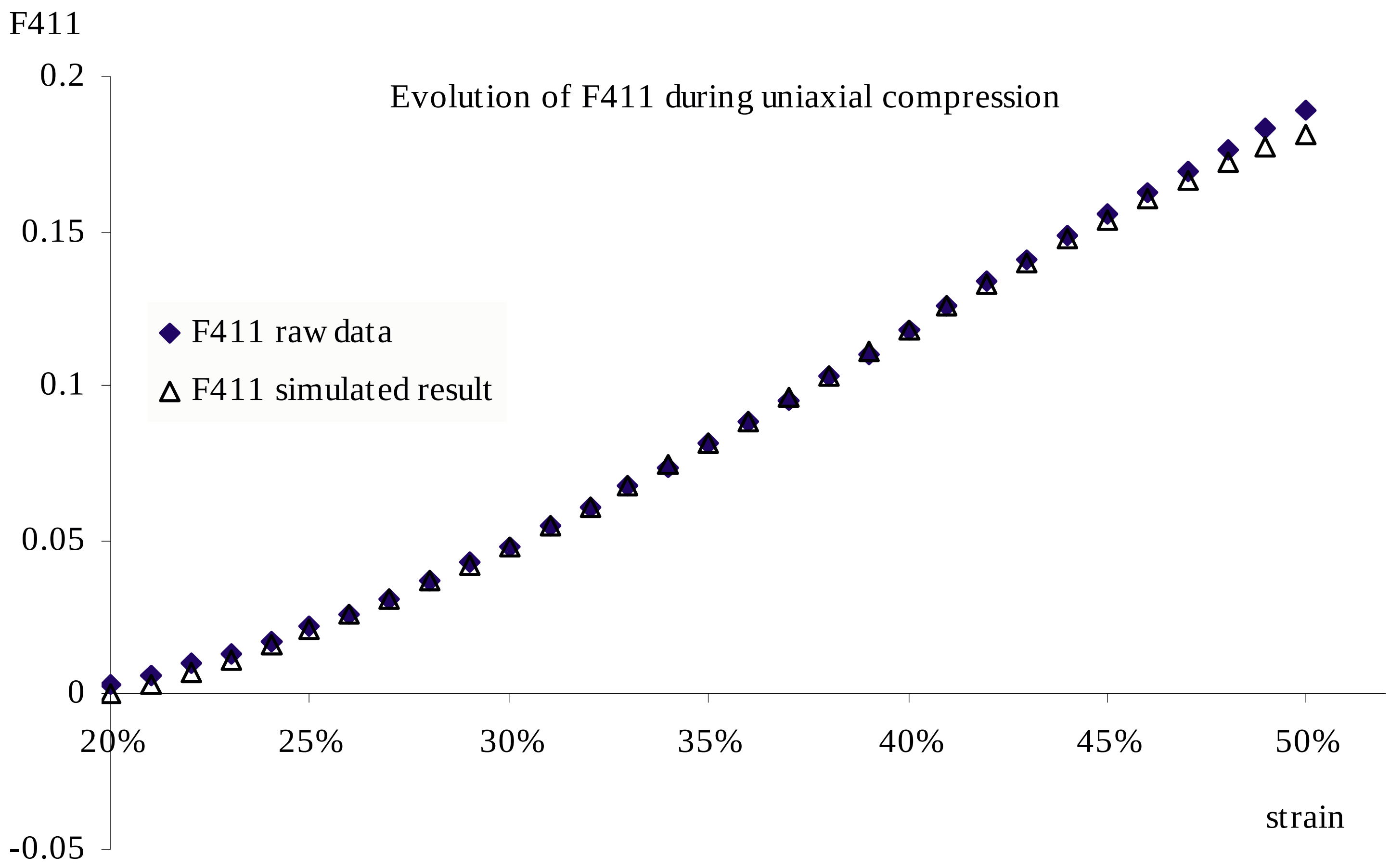
Streamline

Streamline function is obtained by substituting η back to processing path function

$$F(\eta) = \exp\left(\frac{\ln\left(\dfrac{P^{-1}F(\eta)\cdot e^{m}}{P^{-1}F(\eta_0)\cdot e^{m}} \right)}{a_m} A \right) F(\eta_0 = 0)$$

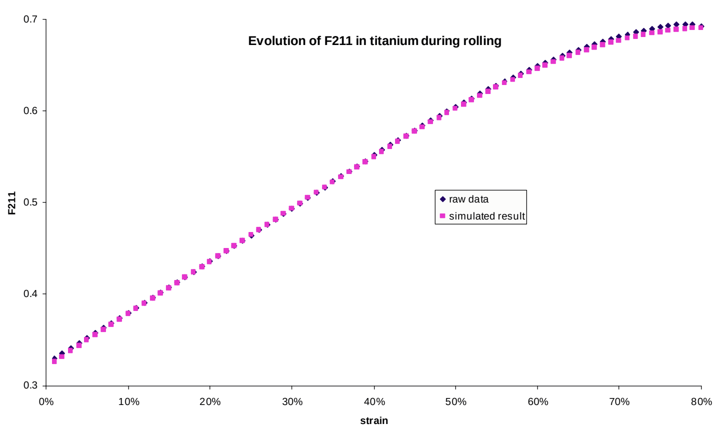


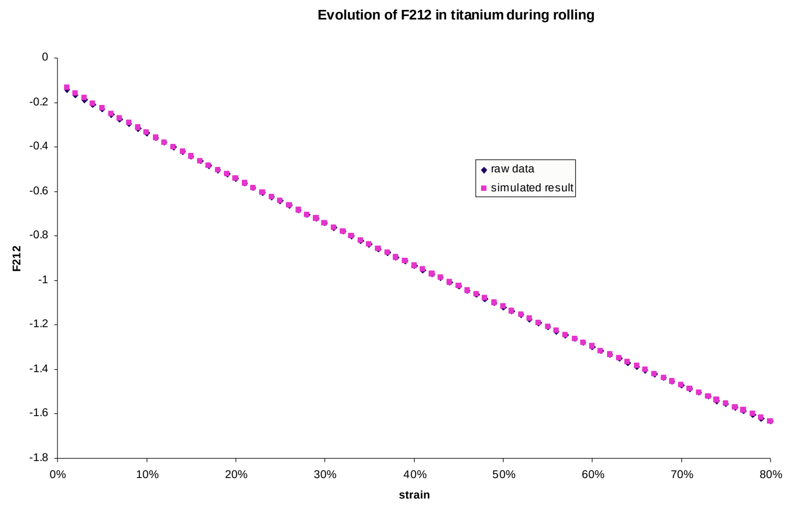
Application of processing path model in other processing method



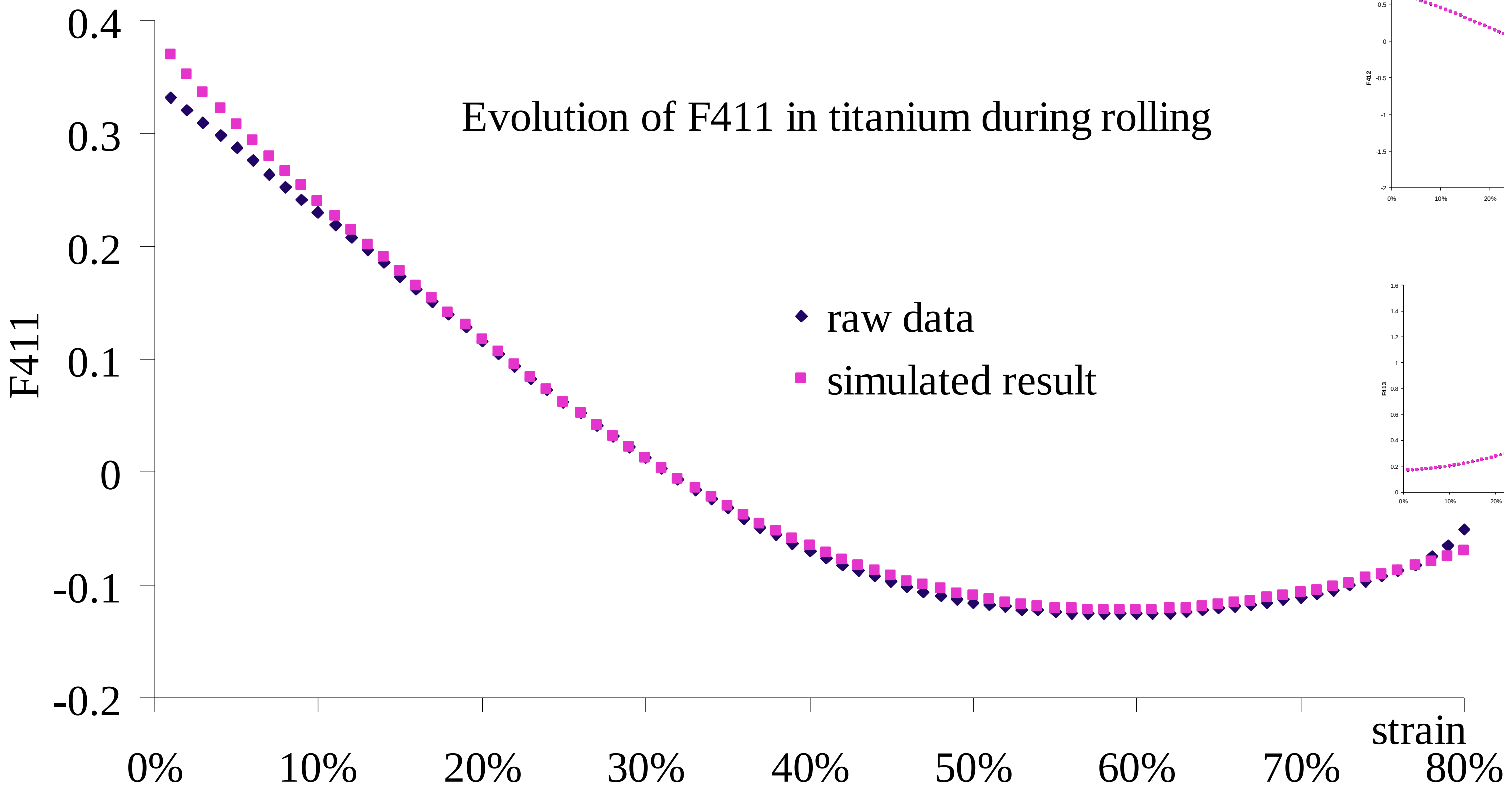
Application of processing path model in Ti (hexagonal)

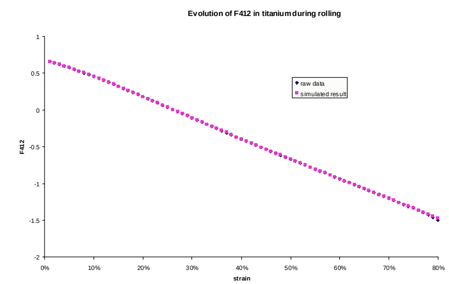
In hexagonal-orthotropic case, 5 nonzero interesting texture coefficients are needed to describe the elastic properties. They are F_2^{11}, F_2^{12}, F_4^{11}, F_4^{12} and F_4^{13}. Texture evolution matrix A is obtained from the raw data. Using A, evolution of the texture coefficients is simulated below:

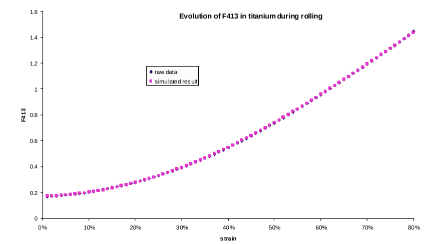




Application of processing path model in Ti (hexagonal)



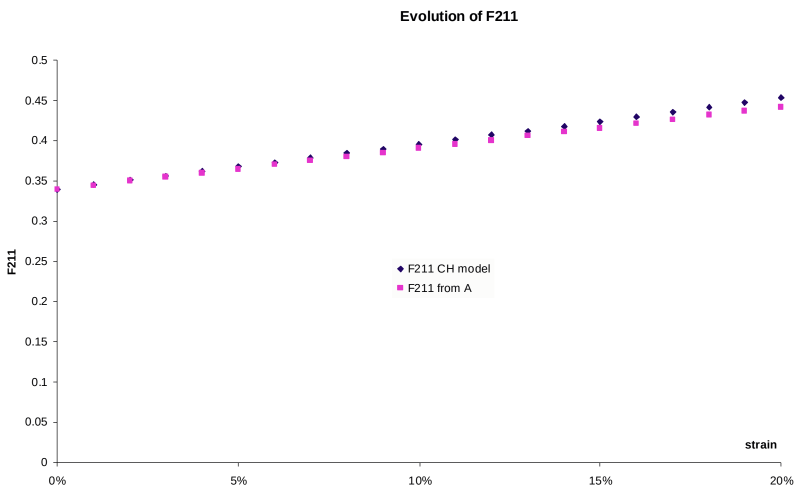


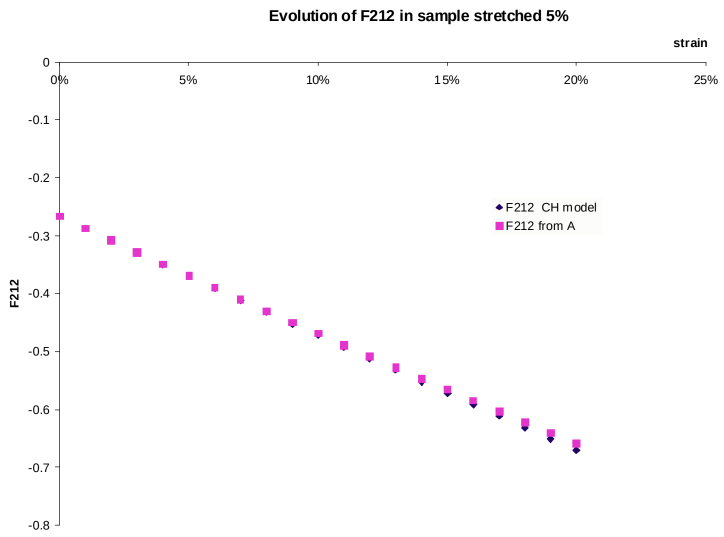


This model not only works in cubic materials, but also works well in hexagonal materials (α phase)

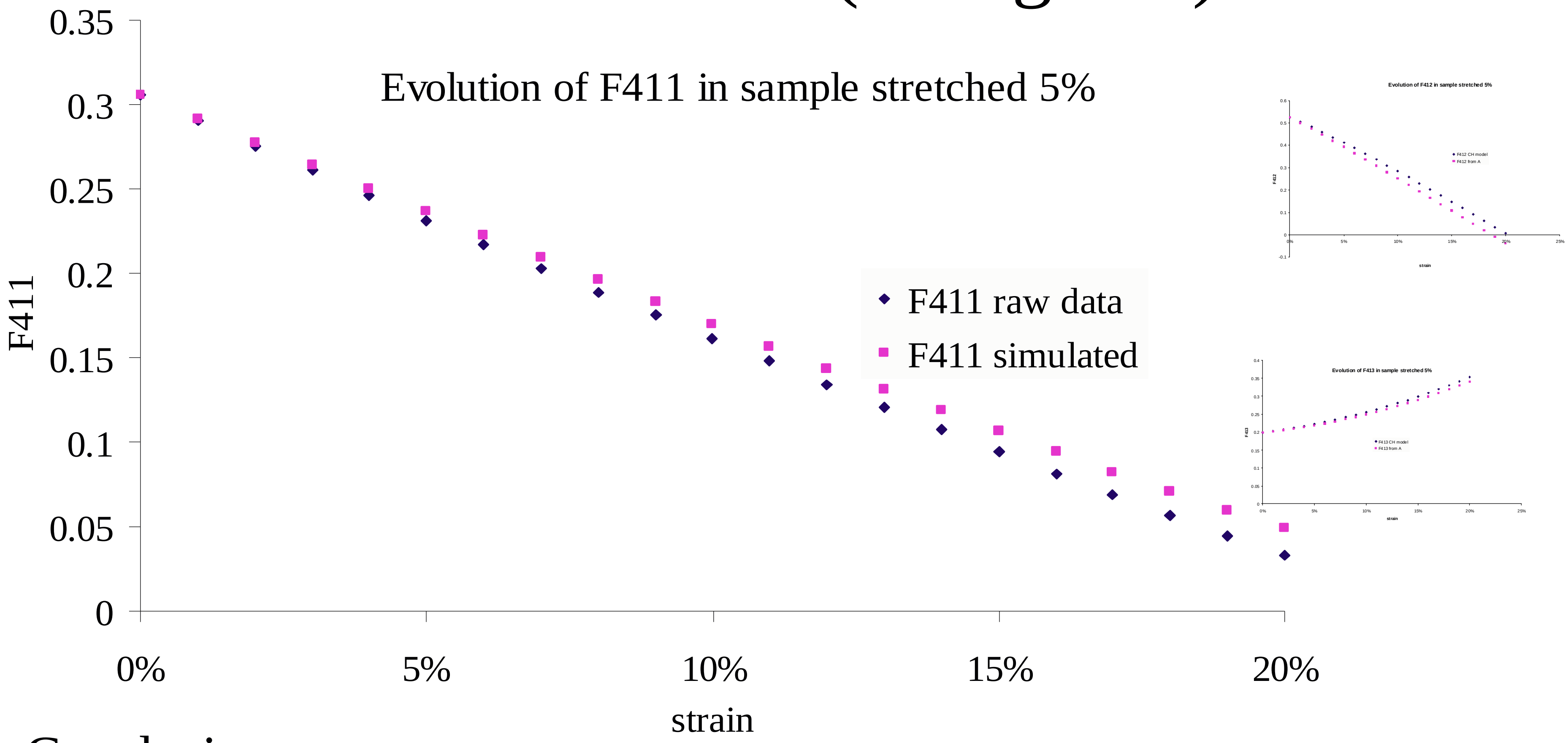
In prediction of texture evolution of Ti (hexagonal)

The obtained texture evolution matrix A is good in rolling. For a sample stretched 5%, apply the same A to simulate the texture evolution during rolling and compare the result from the model:





In prediction of texture evolution of Ti (hexagonal)



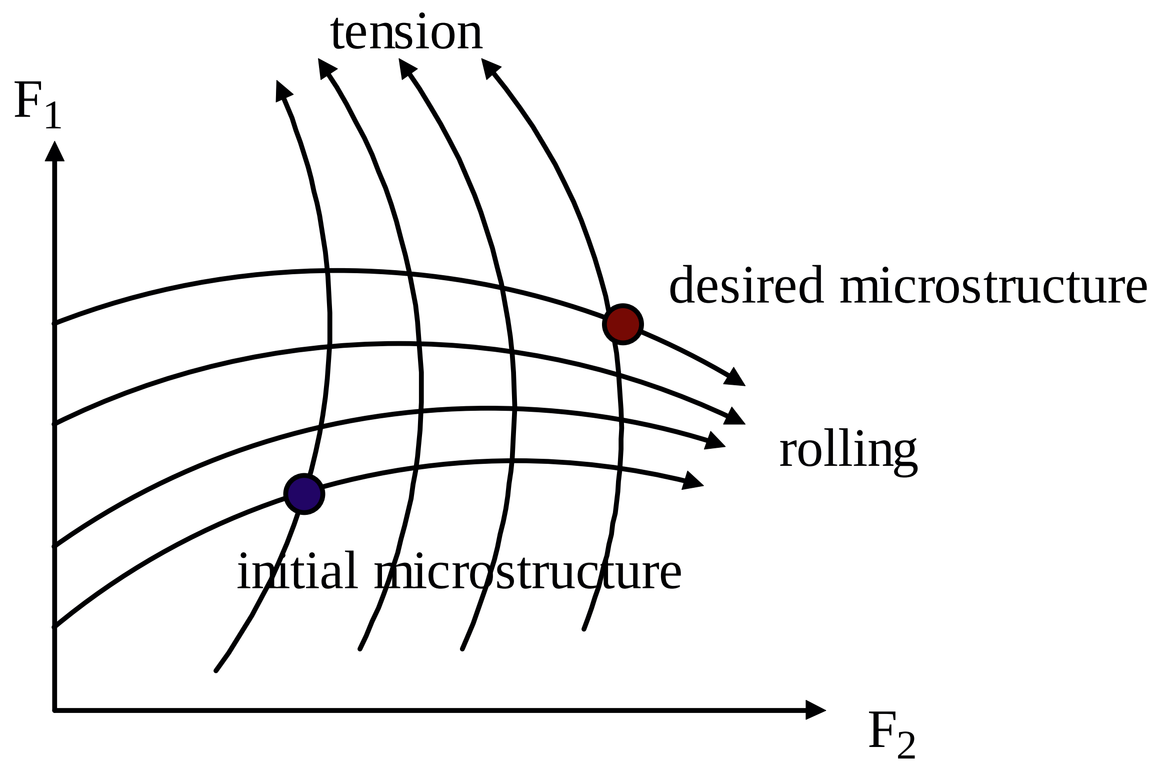
Conclusion:

The prediction using texture evolution matrix A can extrapolate to other microstructure in the material hull.

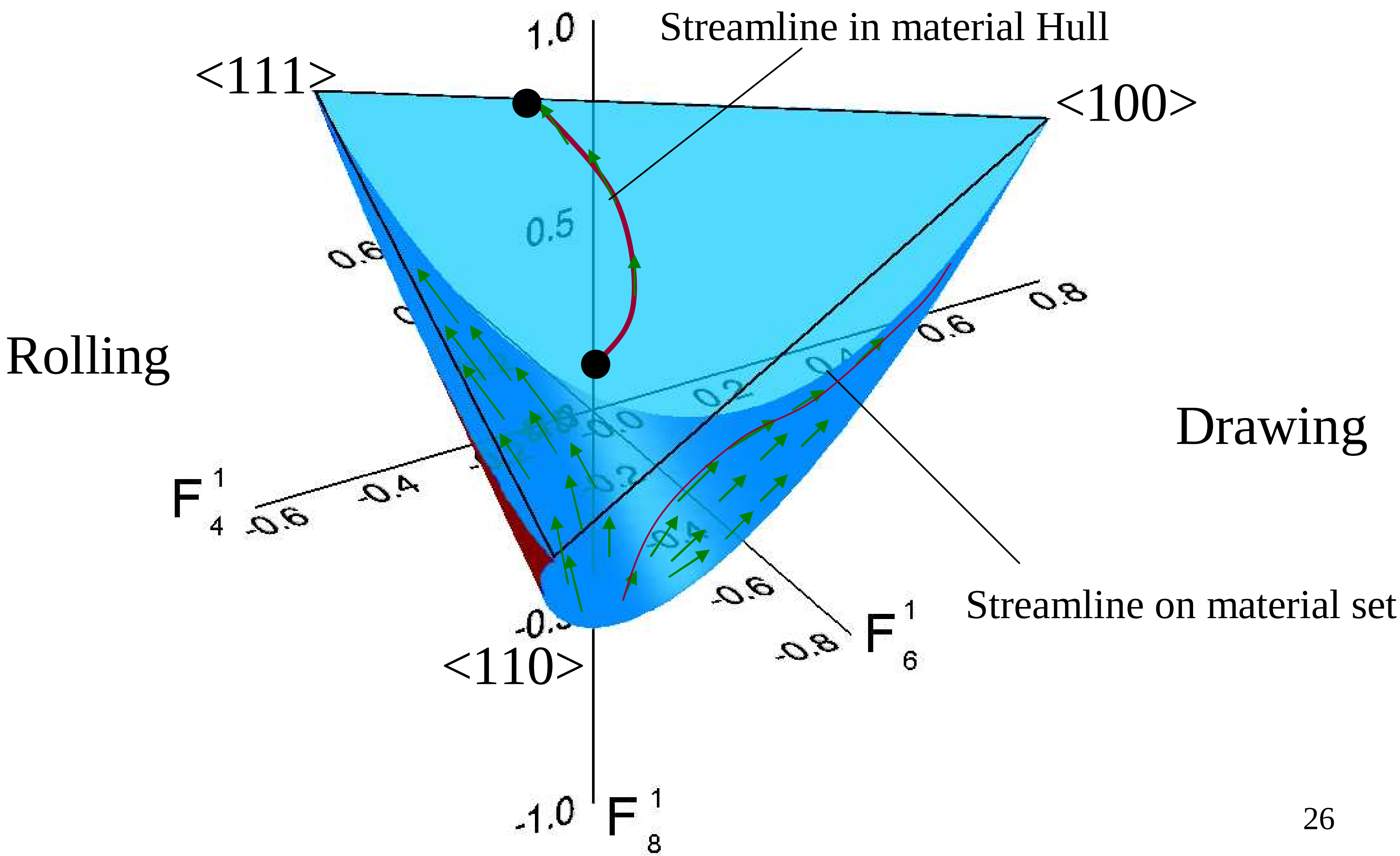
Answer

Q: How to find the processing path from initial microstructure of the raw material to final microstructure with desired properties?

A: Using streamline in processing path model



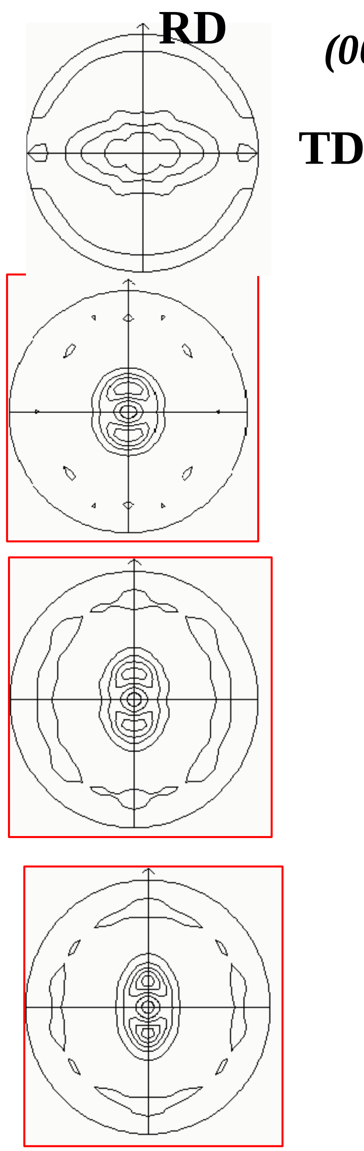
Processing Solutions in Material Space



Simulation of texture evolution in Ti(α) using crystal plasticity model

(0002) Pole Figure Results

Experimental

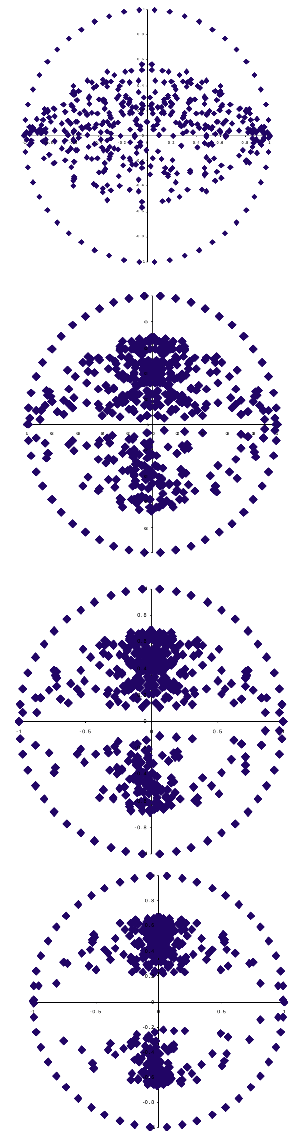


undeformed

Cold Rolled 60%

Cold Rolled 80%

Cold Rolled 95%



Simulated

Processing Path: an Example

strain step=1%, initial strain set includes 29%,30%, 31%, 32%, 33%

strain step=2%, initial strain set includes 26%,28%, 30%, 32%, 34%

strain step=5%, initial strain set includes 25%, 30%, 35%, 40%,45%

least squares error method, initial strains set includes 30%, 31%, 32%,…, 40%

The undeformed texture is random

Uniaxial tension

Using simulated data from Taylor model (crystal plasticity) as raw experimental data

Conclusion

- Any microstructure (texture) is represented by a point in the material hull
- Processing path function and streamline can simulate and predict texture evolution during processing
- Using the streamlines for different processing method can solve and optimize processing path

Thank you!

The End