

**FEM Analysis of
Deformation and Fracture of
Polysynthetically-twinned
 γ -TiAl + α_2 -Ti₃Al Intermetallics**

MS Thesis

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OUTLINE

- **Use of γ -TiAl + α_2 -Ti₃Al Alloys in High-Temperature Structural Applications**
- **Crystal Structures and Slip Systems in γ -TiAl and α_2 -Ti₃Al**
- **Polysynthetically-Twinned γ -TiAl + α_2 -Ti₃Al Single Crystals**
- **Crystal Plasticity Formulation**
- **Determination of Crystal-Plasticity Parameters for γ -TiAl and α_2 -Ti₃Al Single Crystals**
- **Determination of Crystal-Plasticity Parameters for Polysynthetically-Twinned γ -TiAl + α_2 -Ti₃Al Single Crystals**
- **Integration of the Material State**
- **FEM Modeling of Deformation and Fracture in Polycrystalline γ -TiAl + α_2 -Ti₃Al Single Crystals**

Use of

γ -TiAl + α_2 -Ti₃Al Alloys

in High-Temperature

Structural Applications

Favorable High-Temperature Properties:

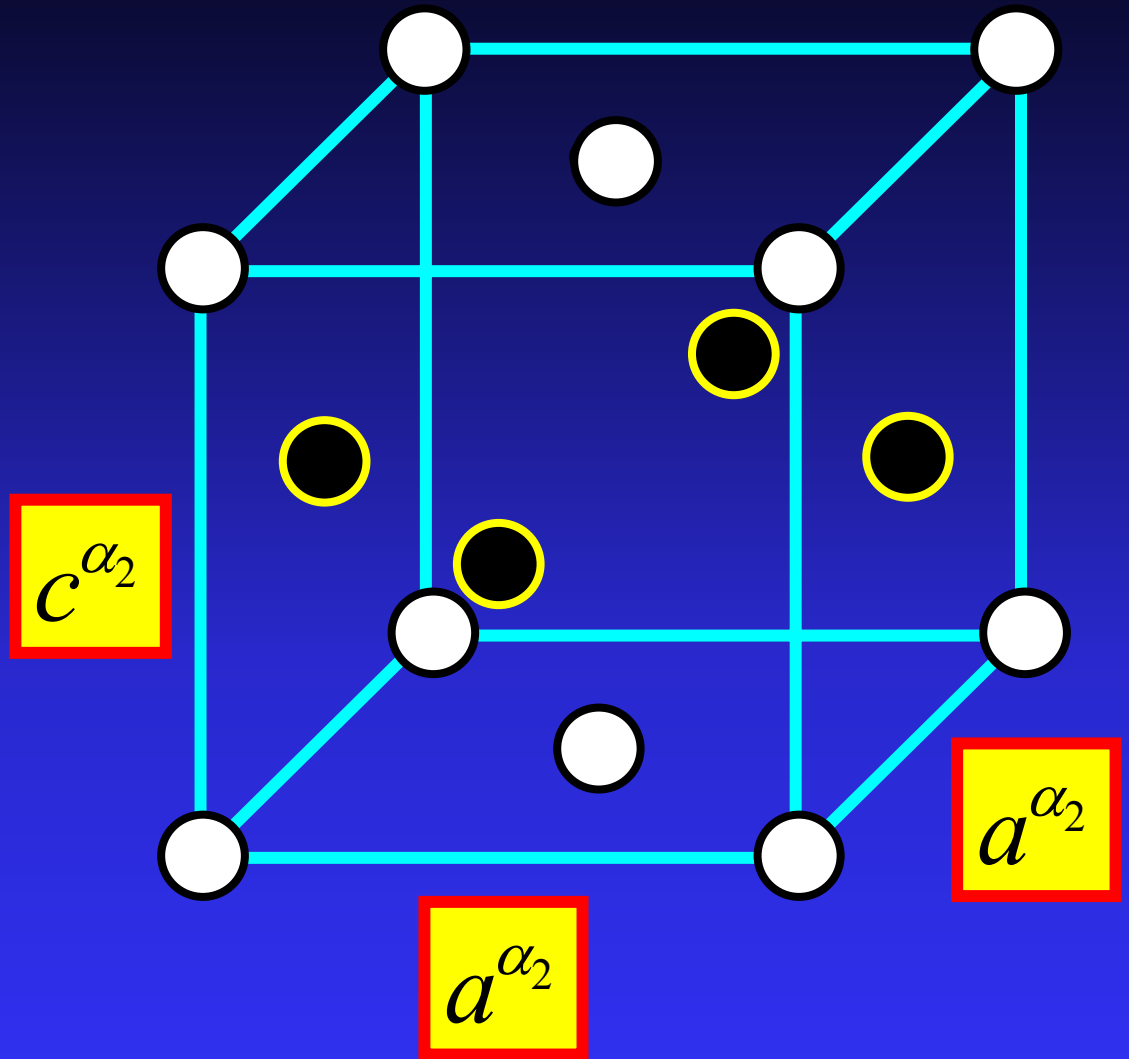
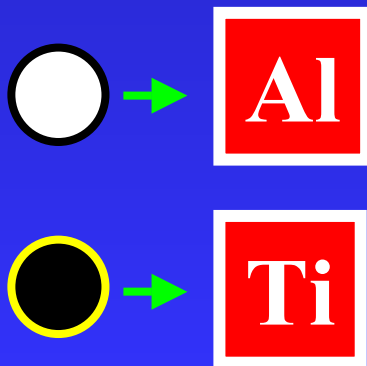
- **Excellent Creep Resistance**
- **Excellent Oxidation Resistance**
- **Light Weight**

Limitations to Applications:

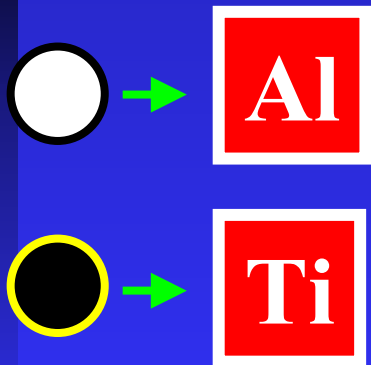
- **Low Ambient-Temperature Ductility**
- **Low Ambient-Temperature Fracture Toughness ($K_{IC} < 30 \text{ MPa}\sqrt{\text{m}}$)**

**Crystal Structures
and
Slip Systems
in
 γ -TiAl and α_2 -Ti₃Al**

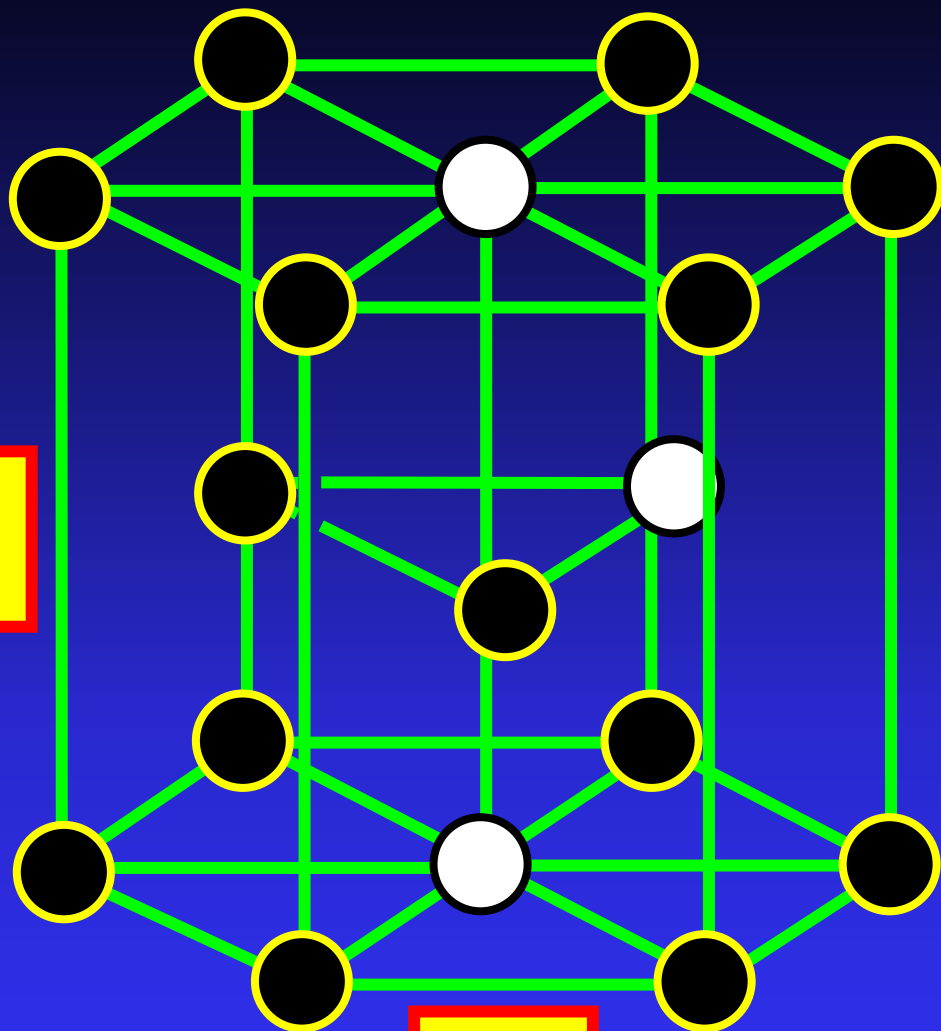
L1₀ γ-TiAl Structure



DO₁₉
 α_2 -Ti₃Al
Structure



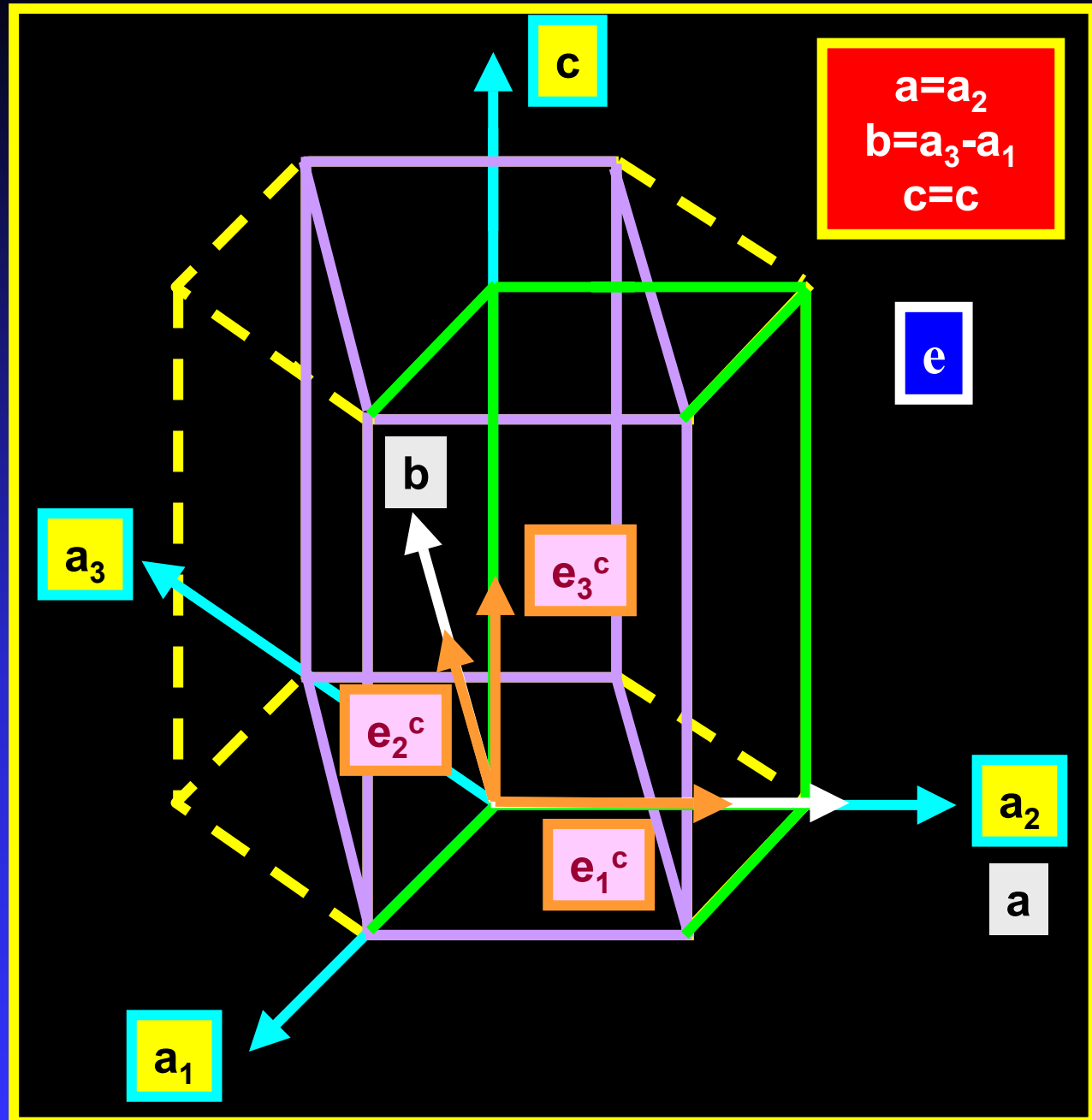
c^{α_2}



a^{α_2}

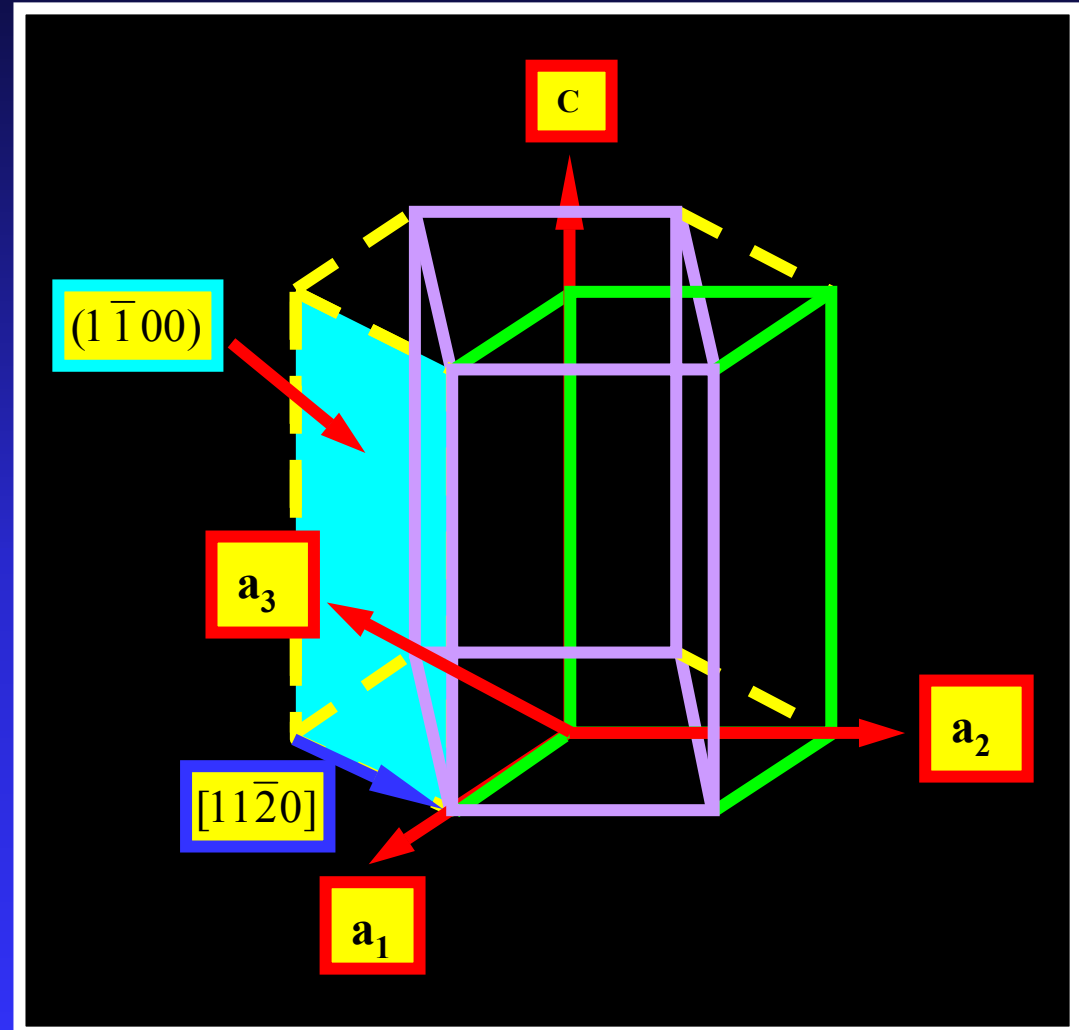
HCP Cell

Simple
Hexagonal
Ortho-
Hexagonal
Prism



Simple
Hexagonal
Ortho-
Hexagonal
Hexagonal
Prism

α_2 -Ti₃Al



Prismatic

$\{10\bar{1}0\} \langle 1\bar{2}10 \rangle$

Slip Systems

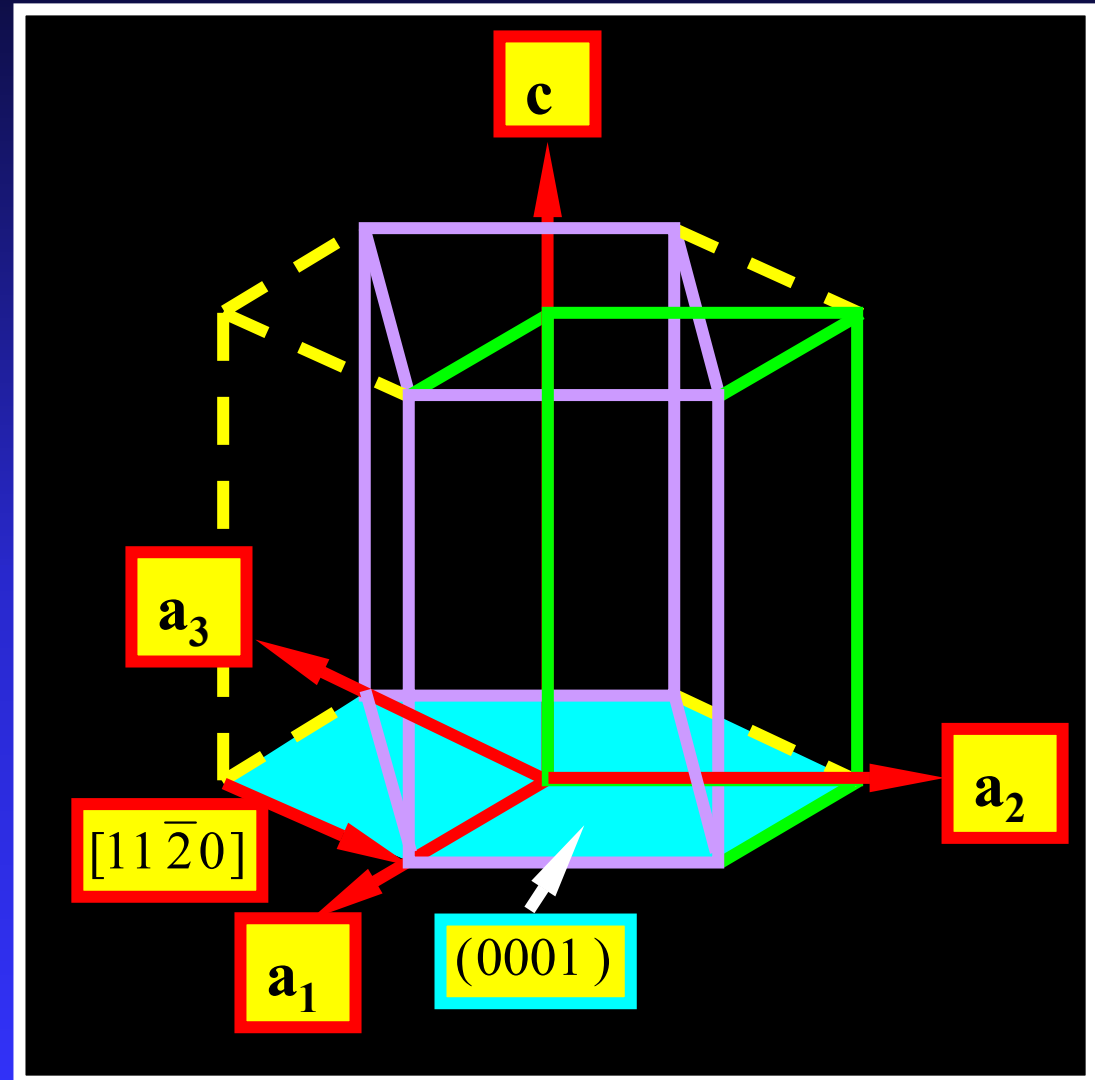
Simple
Hexagonal
Ortho-
Hexagonal
Hexagonal
Prism

$\alpha_2\text{-Ti}_3\text{Al}$

Basal

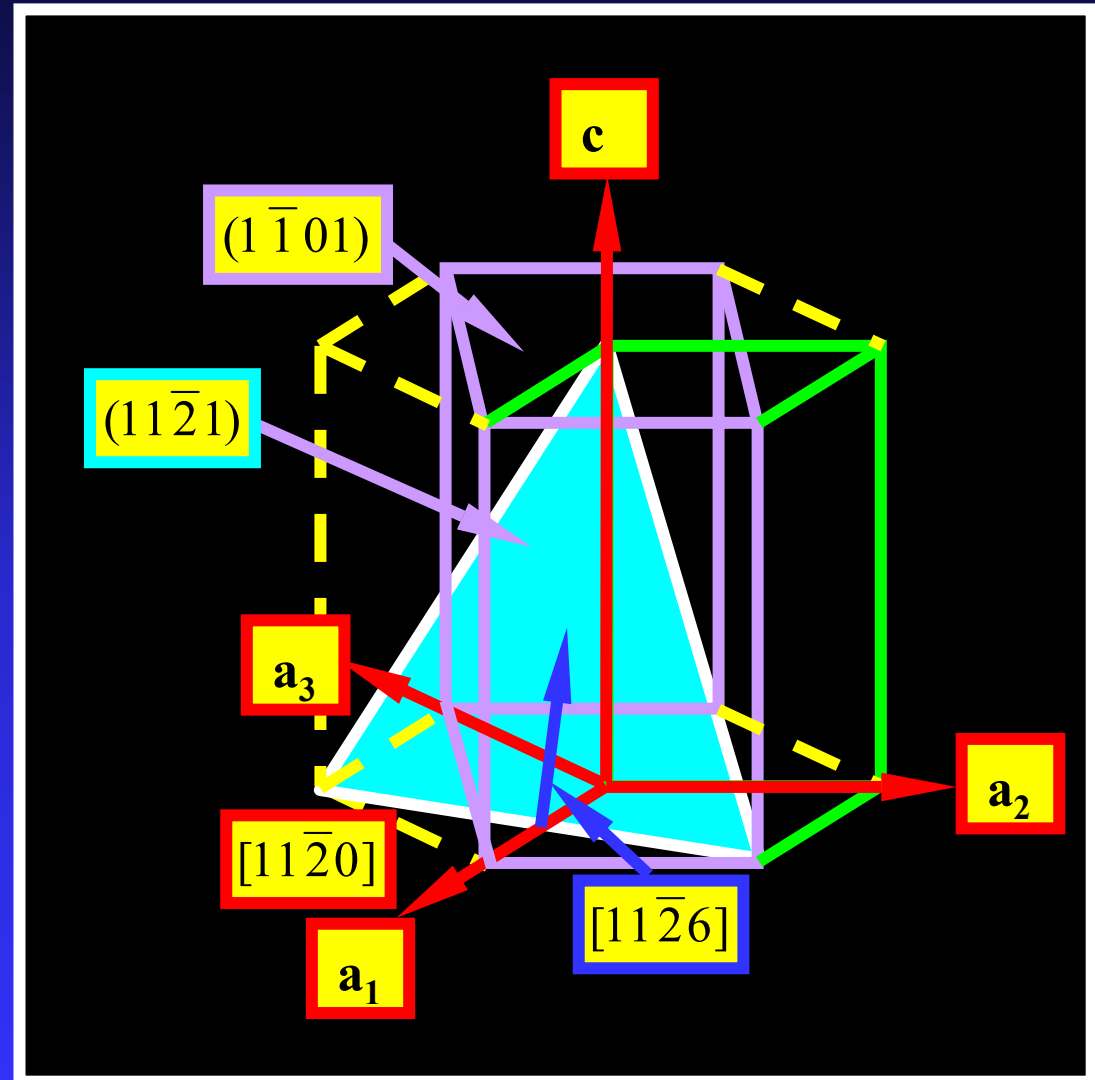
$(0001) \langle 11\bar{2}0 \rangle$

Slip Systems



Simple
Hexagonal
Ortho-
Hexagonal
Hexagonal
Prism

α_2 -Ti₃Al



Pyramidal

$\{11\bar{2}1\} \langle 11\bar{2}6 \rangle$

Slip Systems

Polysynthetically-

Twinned

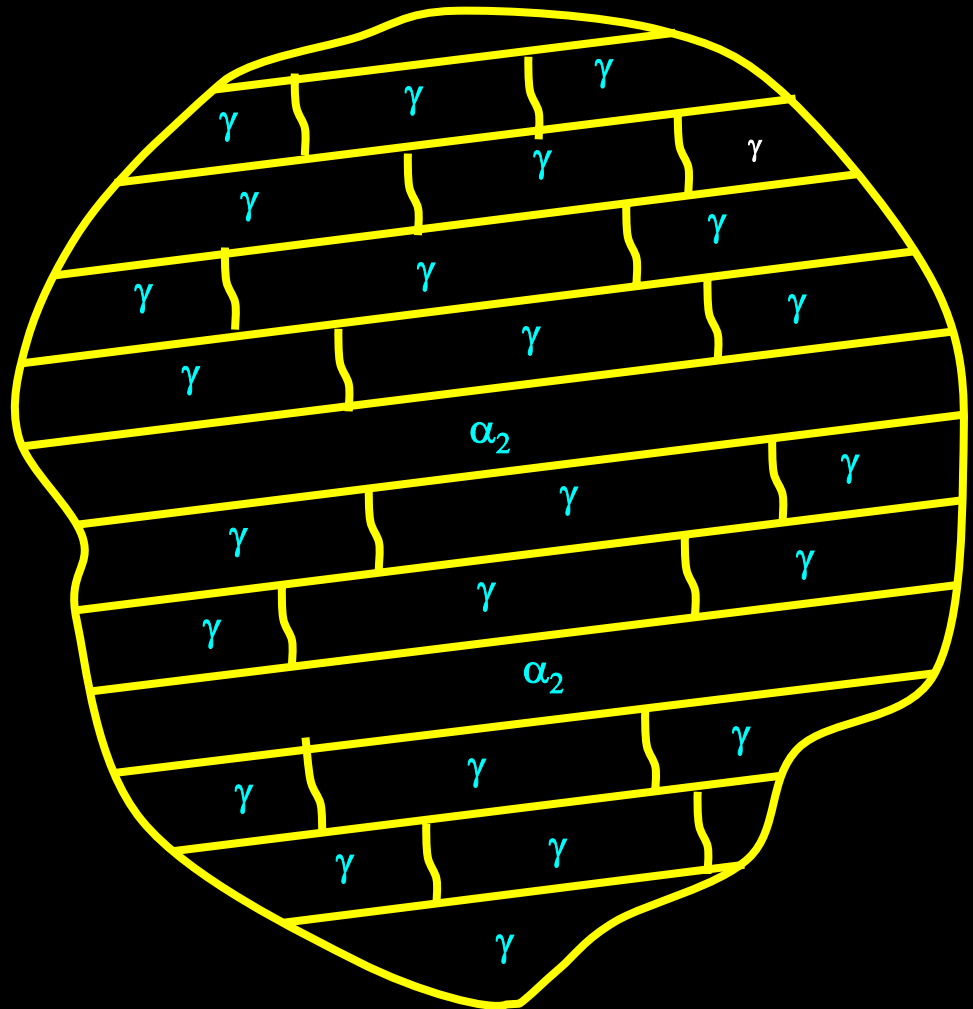
γ -TiAl + α_2 -Ti₃Al

Single Crystals

**Polysynthetically-
twinned
 γ -TiAl+ α_2 -Ti₃Al
Single Crystals**

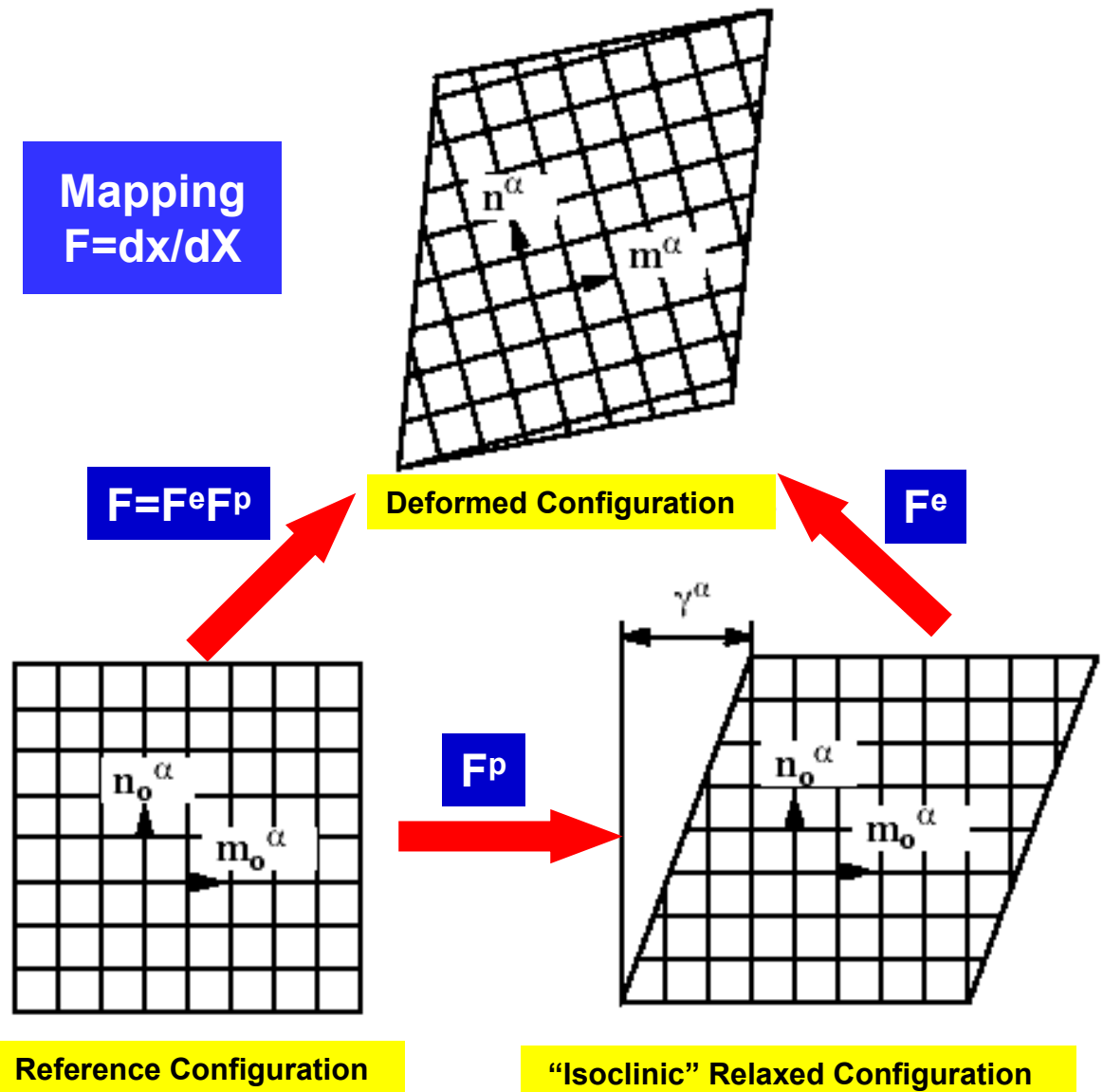
$$\{111\}_{\gamma} \parallel (0001)_{\alpha_2}$$

$$\langle 1\bar{1}0 \rangle_{\gamma} \parallel \langle 11\bar{2}0 \rangle_{\alpha_2}$$



Crystal Plasticity Formulation

Materials Constitutive Model



Materials Constitutive Model, cont'd.

Multiplicative Decomposition of Deformation Gradient

$$F^e \equiv FF^{p-1}, \quad \det F^e > 0$$

Stress vs. Strain Relationship

$$T^* = C[E^e]$$

Stress and Strain Definitions

$$E^e \equiv (1/2)\{F^{eT}F^e - I\} \quad T^* \equiv (\det F^e)F^{e-1}TF^{e-T}$$

Materials Constitutive Model, cont'd.

Elasticity Tensor for γ -TiAl Phase

Six Independent Non-Zero Components

$$C_{11}=C_{22}, C_{33}, C_{12}, C_{13}=C_{23}, C_{44}=C_{55}, C_{66}$$

Elasticity Tensor for α_2 -Ti₃Al Phase

Six Different (Five Independent) Non-Zero Components

$$C_{11}=C_{22}, C_{33}, C_{12}, C_{23}=C_{13}, C_{44}=C_{55}, \\ C_{66}=0.5(C_{11}-C_{12})$$

Materials Constitutive Model, cont'd.

Definition of Slip Plane Normal and Slip Direction Components

For a $\{h\ k\ l\} \langle u\ v\ w \rangle$ slip system in $\gamma\text{-TiAl}$

$$\{n_{0,1}^\alpha, n_{0,2}^\alpha, n_{0,3}^\alpha\} = \left\{ h/a^\gamma, k/a^\gamma, l/a^\gamma \right\} / \left| \left\{ h/a^\gamma, k/a^\gamma, l/a^\gamma \right\} \right|;$$
$$\langle m_{0,1}^\alpha, m_{0,2}^\alpha, m_{0,3}^\alpha \rangle = \langle ua^\gamma, va^\gamma, wa^\gamma \rangle / \left| \langle ua^\gamma, va^\gamma, wa^\gamma \rangle \right|.$$

For a $\{h\ k\ m\ l\} \langle u\ v\ z\ w \rangle$ slip system in $\alpha_2\text{-Ti}_3\text{Al}$

$$\{n_{0,1}^\alpha, n_{0,2}^\alpha, n_{0,3}^\alpha\} = \left\{ k, -(k+2h)/\sqrt{3}, l/(c^{\alpha_2}/a^{\alpha_2}) \right\} /$$
$$\left| \left\{ k, -(k+2h)/\sqrt{3}, l/(c^{\alpha_2}/a^{\alpha_2}) \right\} \right|;$$
$$\langle m_{0,1}^\alpha, m_{0,2}^\alpha, m_{0,3}^\alpha \rangle = \langle 3v/2, -\sqrt{3}(u+v/2), w(c^{\alpha_2}/a^{\alpha_2}) \rangle /$$
$$\left| \langle 3v/2, -\sqrt{3}(u+v/2), w(c^{\alpha_2}/a^{\alpha_2}) \rangle \right|.$$

Materials Constitutive Model, cont'd.

Evolution Equation for Plastic Deformation Gradient

$$\dot{F}^p F^{p-1} = \sum_{\beta} \dot{\gamma}^{\beta} S_0^{\beta} \quad S_0^{\alpha} \equiv m_0^{\alpha} \otimes n_0^{\alpha}$$

Shearing Rate on Slip System α

$$\dot{\gamma}^{\alpha} = \tilde{\gamma} \frac{|\tau^{\alpha}|^{1/m}}{|S^{\alpha}|} \text{sign}(\tau^{\alpha})$$

Resolved Shear Stress

$$\tau^{\alpha} \equiv T^* \cdot S_0^{\alpha}$$

Materials Constitutive Model, cont'd.

Shear Resistance Evolution Equation

$$\dot{s}^{\alpha} = \sum_{\beta} h^{\alpha\beta} |\dot{\gamma}^{\beta}|$$

Hardening Rate Matrix

$$h^{\alpha\beta} = q^{\alpha\beta} h^{\beta}$$

Self Hardening Rate

$$h^{\beta} = h_0^{\beta} \left| 1 - \frac{s^{\beta}}{s_s^{\beta}} \right|^r \operatorname{sign} \left(1 - \frac{s^{\beta}}{s_s^{\beta}} \right)$$

Materials Constitutive Model, cont'd.

Latent Hardening Rate

$$q^{\alpha\beta} = \begin{cases} 1 & \text{if } \alpha \text{ and } \beta \text{ are coplanar slip systems} \\ q_l & \text{otherwise} \end{cases}$$

Coplanar Slip Systems in the Two Phases

γ - TiAl Phase : One $\{111\} \langle 1\bar{1}0 \rangle$, two $\{111\} \langle 0\bar{1}1 \rangle$, one $\{111\} [11\bar{2}]$ slip systems
 α_2 - Ti_3Al Phase : Three basal $\langle a \rangle$ -slip systems : $(0001)[11\bar{2}0]$, $(0001)[\bar{2}110]$,
 $(0001)[1\bar{2}10]$

**Determination of
Crystal-Plasticity
Parameters for
 γ -TiAl and α_2 -Ti₃Al
Single Crystals**

Results

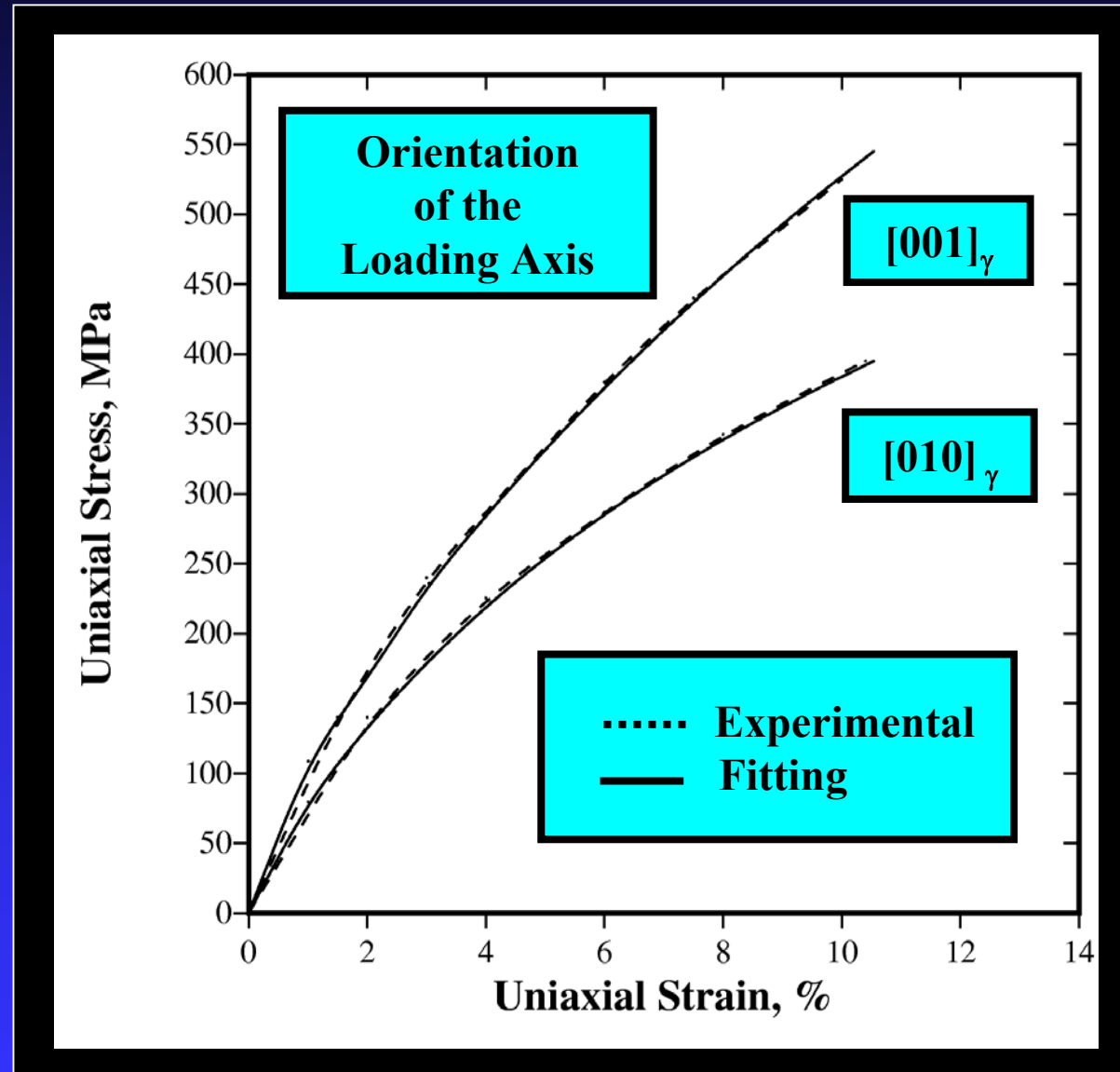
Crystallographic Parameters for Five γ -TiAl Single-Crystal Orientations Used in the Work of Kawabata et al.

Orientation of Compression Axis	Slip Systems with Maximum Initial Schmid Factor	Magnitude of Schmid Factor
$[001]$	Eight $\langle 10\bar{1} \rangle \{111\}$	~ 0.409
$[\bar{1}10]$	Four $\langle 10\bar{1} \rangle \{111\}$	~ 0.409
$[010]$	Four $\langle 1\bar{1}0 \rangle \{111\}$ Four $\langle 10\bar{1} \rangle \{111\}$	~ 0.409
$\sim [\bar{2}96]$	Single $[1\bar{1}0](111)$	~ 0.482
$\sim [\bar{2}45]$	Single $[10\bar{1}](111)$	~ 0.445

Results Cont'd.

γ -TiAl Single Crystals

Curve Fitting



Results Cont'd.

Crystal-Plasticity Parameters for the γ -TiAl Single Crystals

Parameter	Symbol	Value	Units	Reference
Elastic Constant	C_{11}	190	GPa	(22)
Elastic Constant	C_{33}	185	GPa	(22)
Elastic Constant	C_{12}	105	GPa	(22)
Elastic Constant	C_{13}	90	GPa	(22)
Elastic Constant	C_{44}	120	GPa	(22)
Elastic Constant	C_{66}	50	GPa	(22)
Reference Shearing Rate	$\dot{\gamma}_0$	0.005	s^{-1}	This Work
Strain Rate Sensitivity	m	0.014	N/A	This Work
Latent Hardening Parameter	q_i	1.4	N/A	This Work

Table Cont'd. ↓

Results Cont'd.

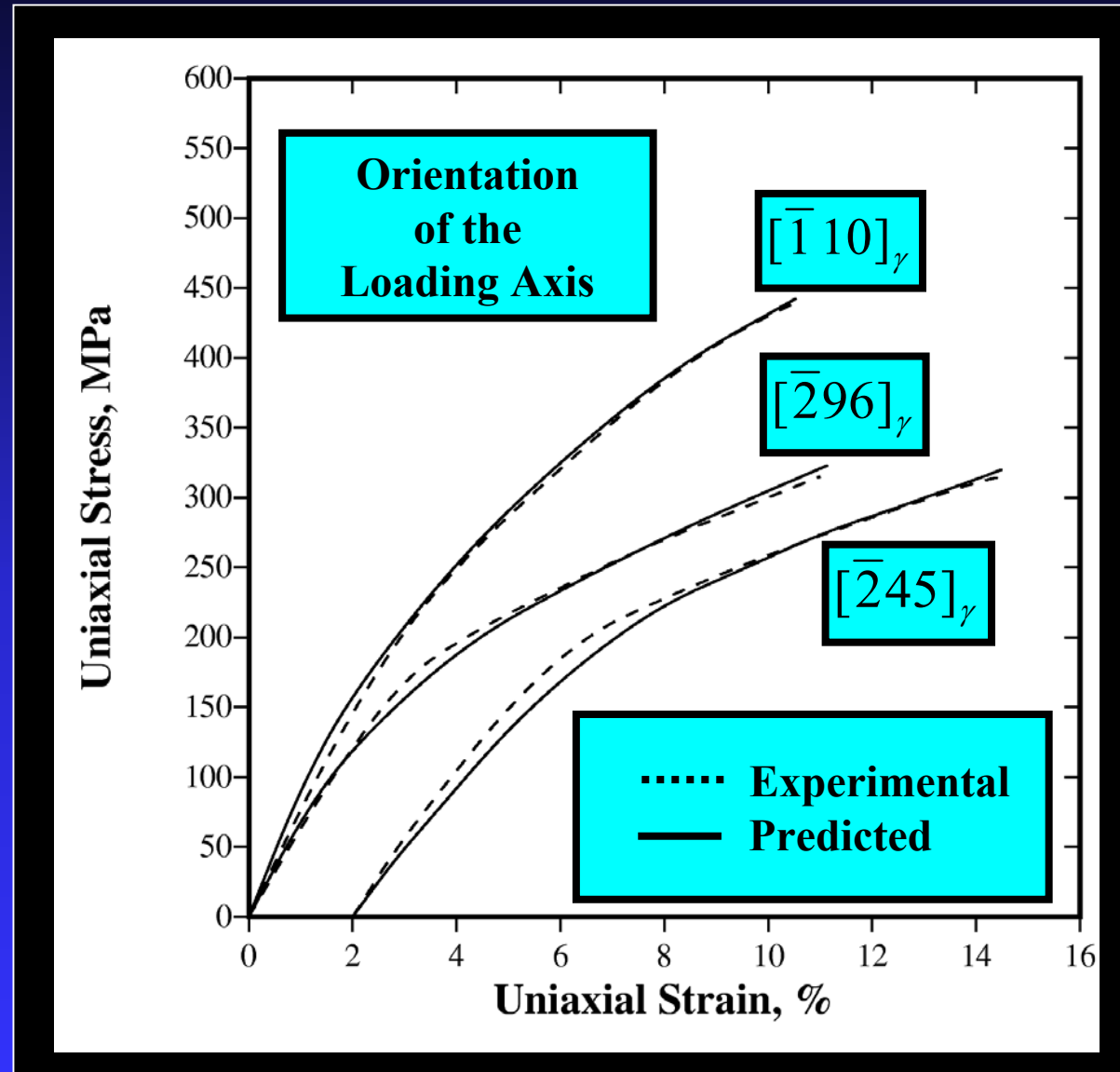
Table Cont'd.

Self-Hardening Exponent	$\{11\} 1/2 \langle \bar{1}\bar{1}0 \rangle$	r	3.1	N/A	This Work
	$\{11\} \langle \bar{1}0\bar{1} \rangle$		3.0		
Initial Slip Resistance	$\{11\} 1/2 \langle \bar{1}\bar{1}0 \rangle$	s_0	14.3	Mpa	This Work
	$\{11\} \langle \bar{1}0\bar{1} \rangle$		22.7		
Self-Hardening Parameter	$\{11\} 1/2 \langle \bar{1}\bar{1}0 \rangle$	h_0	940.2	Mpa	This Work
	$\{11\} \langle \bar{1}0\bar{1} \rangle$		950.7		
Saturation Slip Resistance	$\{11\} 1/2 \langle \bar{1}\bar{1}0 \rangle$	s_s	212.2	MPa	This Work
	$\{11\} \langle \bar{1}0\bar{1} \rangle$		291.1		

Results Cont'd.

γ -TiAl Single Crystals

Predicted Curves



Results

Crystallographic Parameters for the α_2 -Ti₃Al Single Crystals
Used in the Work of Inui et al.

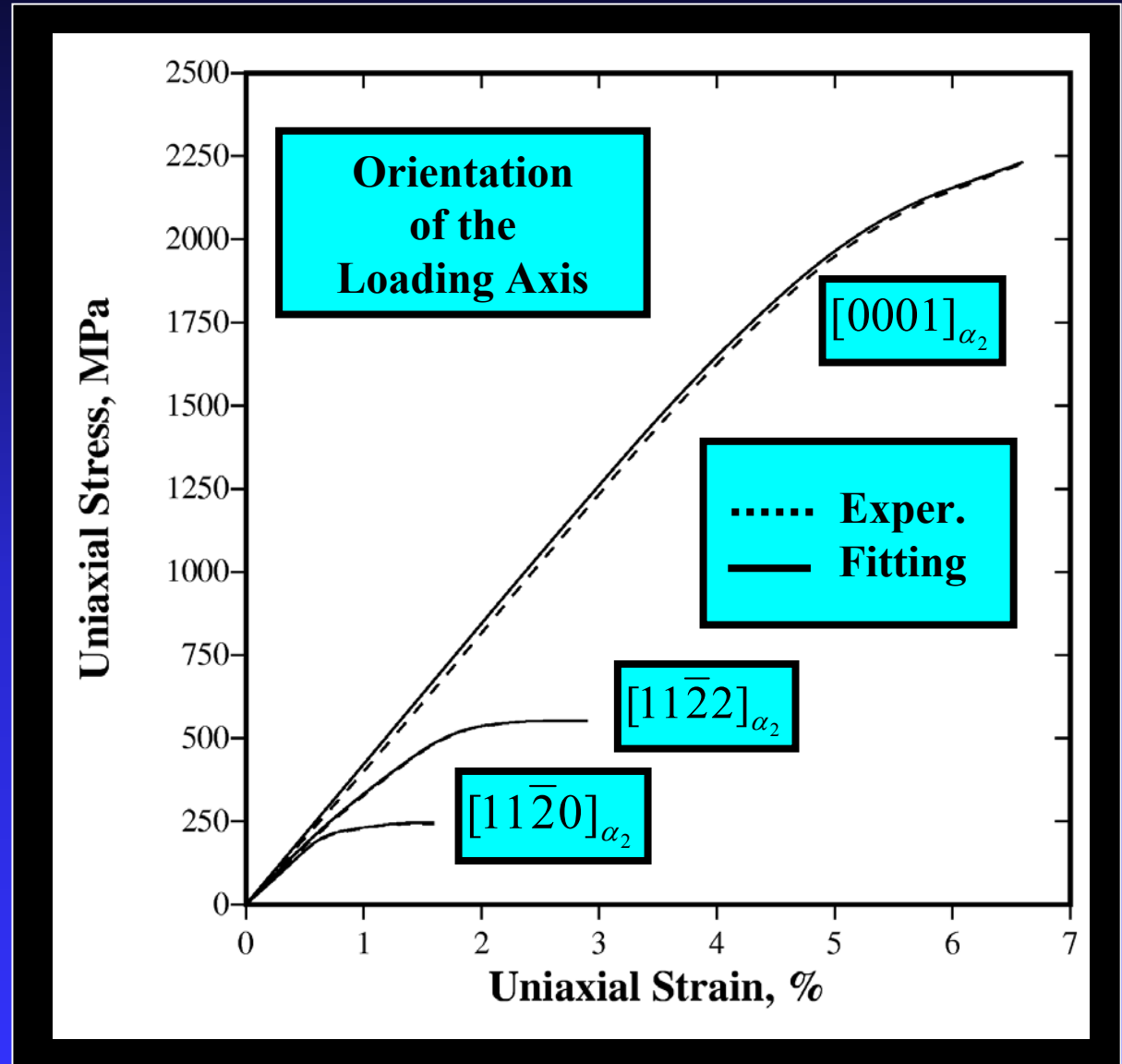
$$\omega = \phi = 0, 0 \leq \theta \leq 90^\circ$$

Single-Crystal Orientation		Magnitude of Schmid Factor		
Orientation of Compression Axis	Euler Angle, θ	(0001) $\langle 11\bar{2}0 \rangle$ Basal Slip	(1 $\bar{1}$ 00) $\langle 11\bar{2}0 \rangle$ Prismatic Slip	(11 $\bar{2}$ 1) $\langle \bar{1}\bar{1}26 \rangle$ Pyramidal Slip
[0001]	0	0	0	0.4494
[11 $\bar{2}$ 4]	22	0.3449	0.0619	0.4459
[11 $\bar{2}$ 2]	39	0.4889	0.1732	0.3321
[11 $\bar{2}$ 1]	59	0.4454	0.3149	0.3995
[11 $\bar{2}$ 0]	90	0	0.4330	0.4494

Results Cont'd.

α_2 -Ti₃Al
Single
Crystals

Curve
Fitting



Results Cont'd.

Crystal-Plasticity Parameters for the α_2 -Ti₃Al Single Crystals

Parameter	Symbol	Value	Units	Reference
Elastic Constant	C_{11}	221	GPa	(23)
Elastic Constant	C_{33}	238	GPa	(23)
Elastic Constant	C_{12}	71	GPa	(23)
Elastic Constant	C_{13}	85	GPa	(23)
Elastic Constant	C_{44}	69	GPa	(23)
Reference Shearing Rate	$\dot{\gamma}_0$	0.001	s ⁻¹	This Work
Strain Rate Sensitivity	m	0.009	N/A	This Work
Latent Hardening Parameter	q_1	1.4	N/A	This Work

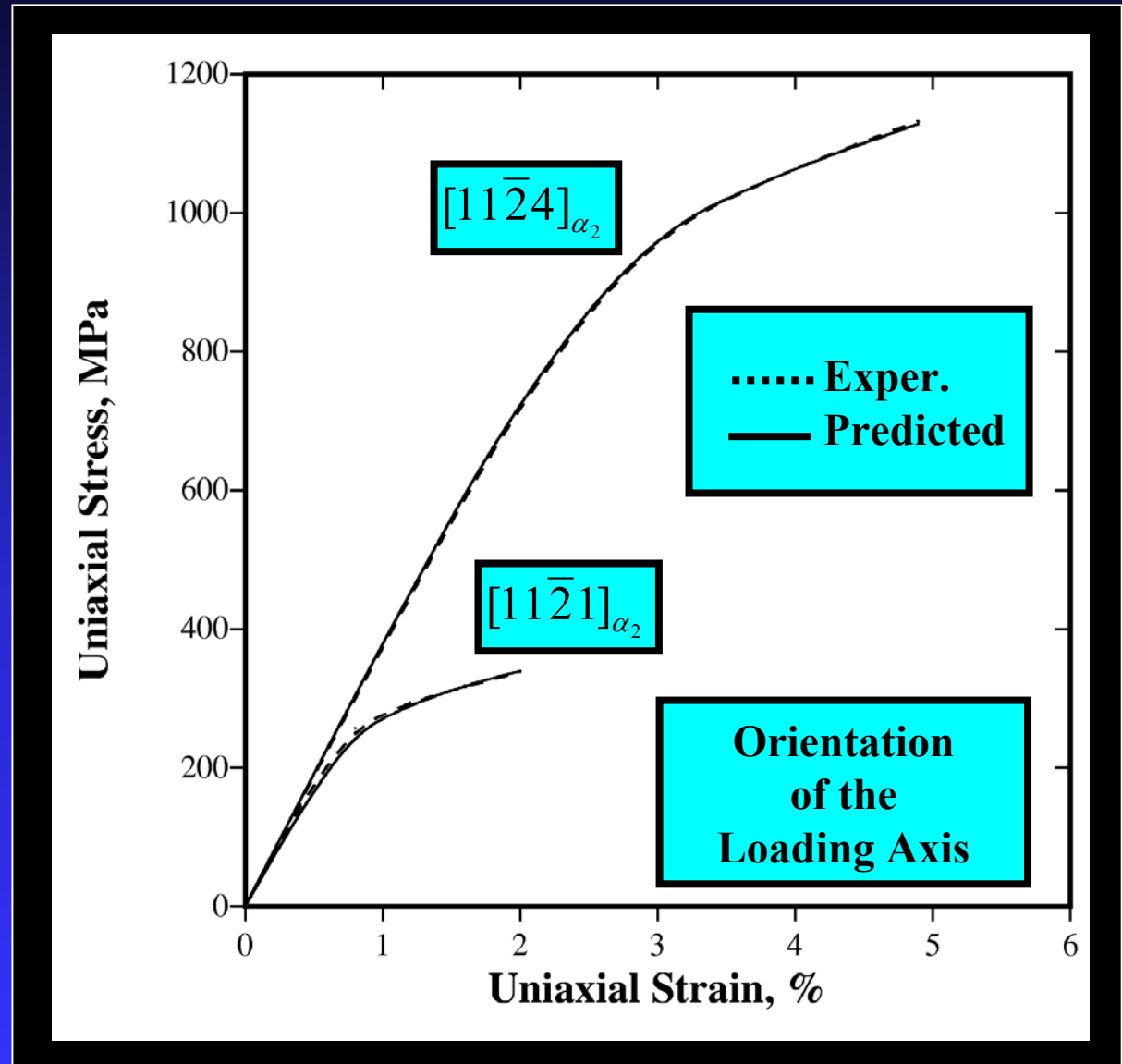
Table Cont'd. ↓

Self-Hardening Exponent	$\{1\bar{1}00\} \langle 1\bar{1}20 \rangle$	r	2.7	N/A	This Work
	$\{0001\} \langle 1\bar{1}20 \rangle$		3.0		
	$\{1\bar{1}21\} \langle 1\bar{1}26 \rangle$		2.9		
Initial Slip Resistance	$\{1\bar{1}00\} \langle 1\bar{1}20 \rangle$	s₀	19.2	MPa	This Work
	$\{0001\} \langle 1\bar{1}20 \rangle$		44.8		
	$\{1\bar{1}21\} \langle 1\bar{1}26 \rangle$		121.9		
Self-Hardening Parameter	$\{1\bar{1}00\} \langle 1\bar{1}20 \rangle$	h₀	861.7	MPa	This Work
	$\{0001\} \langle 1\bar{1}20 \rangle$		742.8		
	$\{1\bar{1}21\} \langle 1\bar{1}26 \rangle$		814.7		
Saturation Slip Resistance	$\{1\bar{1}00\} \langle 1\bar{1}20 \rangle$	s_s	149.3	MPa	This Work
	$\{0001\} \langle 1\bar{1}20 \rangle$		417.7		
	$\{1\bar{1}21\} \langle 1\bar{1}26 \rangle$		1586.3		

Results Cont'd.

α_2 -Ti₃Al
Single
Crystals

Predicted
Curves



**Determination of
Crystal-Plasticity
Parameters for
Polysynthetically-Twinned
 γ -TiAl + α_2 -Ti₃Al
Single Crystals**

Results Cont'd.

γ -TiAl +
 α_2 -Ti₃Al
Single
Crystals

Slip System	Symbol	Slip Type
$[1\bar{1}0](111)$	S1	Soft Mode
$[\bar{1}01](111)$		
$[01\bar{1}](111)$		
$[\bar{1}01](1\bar{1}1)$	S2	Soft Mode
$[1\bar{1}0](11\bar{1})$		
$[0\bar{1}1](\bar{1}11)$		

Table Cont'd. ↓

Results Cont'd.

γ -TiAl +
 α_2 -Ti₃Al
Single
Crystals

$[1\bar{1}0](111)$

$[\bar{1}01](111)$

$[01\bar{1}](111)$

$[\bar{1}01](1\bar{1}1)$

$[1\bar{1}0](11\bar{1})$

$[0\bar{1}1](\bar{1}11)$

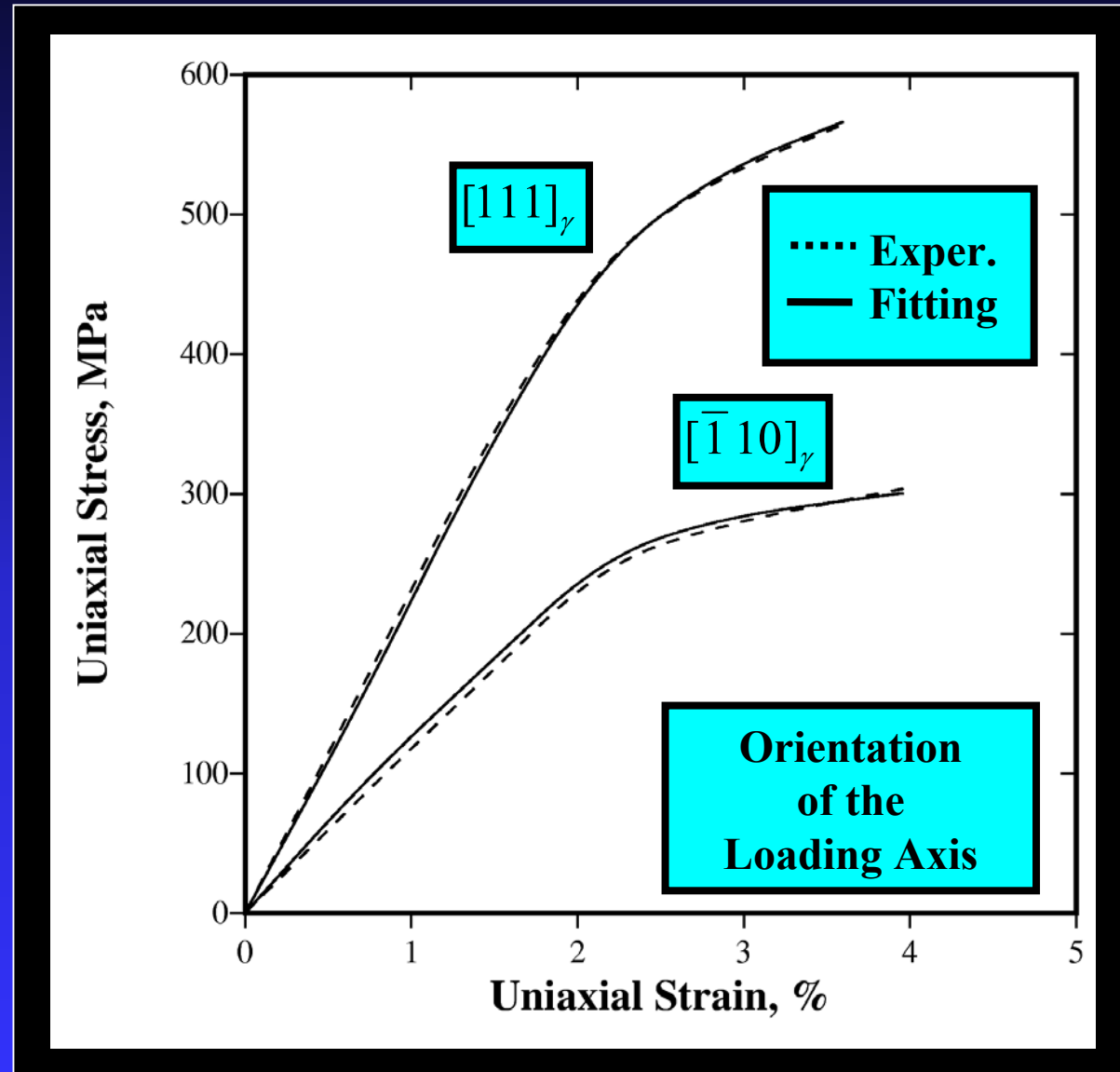
H1

Hard Mode

Results Cont'd.

γ -TiAl +
 α_2 -Ti₃Al
Single
Crystals

Curve
Fitting

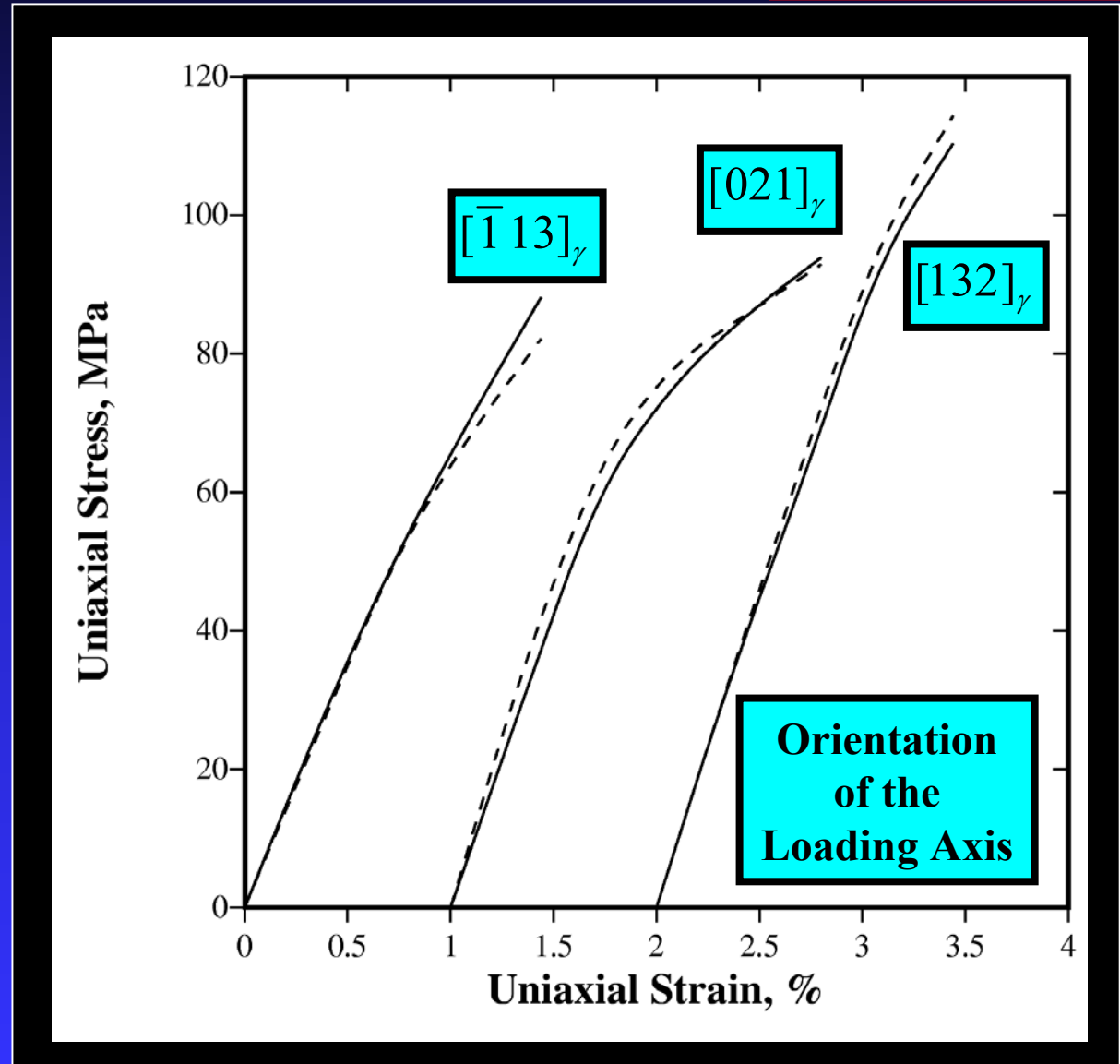


Results Cont'd.

..... Exper.
— Predicted

γ -TiAl +
 α_2 -Ti₃Al
Single
Crystals

Predicted
Curves





**Integration
of the
Material State**

Integration of Material State

(a) Compute $F^{p-1}(\tau)$

$$F^e(t) = F(t)F^{p-1}(t)$$

$$E^e(t) = \frac{1}{2} \{ F^e(t)^T F^e(t) - I \}$$

$$T^*(t) = C(E^*(t))$$

$$\tau^\alpha(t) = T^*(t) \cdot S_0^\alpha$$

Integration of Material State, Cont'd.

$$\dot{\gamma}^{\alpha} = \tilde{\gamma} \frac{|\tau^{\alpha}(t)|^{\frac{1}{m}}}{|s^{\alpha}(t)|} \Delta t$$

$$F^{p^{-1}}(\tau) \cong F^{p^{-1}}(t) \left\{ I - \sum_{\alpha} \Delta \gamma^{\alpha}(t) S_0^{\alpha} \right\}$$

(b) Compute Cauchy Stress $T(\tau)$

$$F^e(\tau) = F(\tau) F^{p^{-1}}(\tau)$$

$$E^e(\tau) = \frac{1}{2} \{ F^e(\tau)^T F^e(\tau) - I \}$$

Integration of Material State, Cont'd.

$$T^*(\tau) = C(E^*(\tau))$$

$$T(\tau) = \det(F^*(\tau))^{-1} F^*(\tau) T^*(\tau) F^*(\tau)^T$$

(c) Update Slip Resistances $s^\alpha(\tau)$

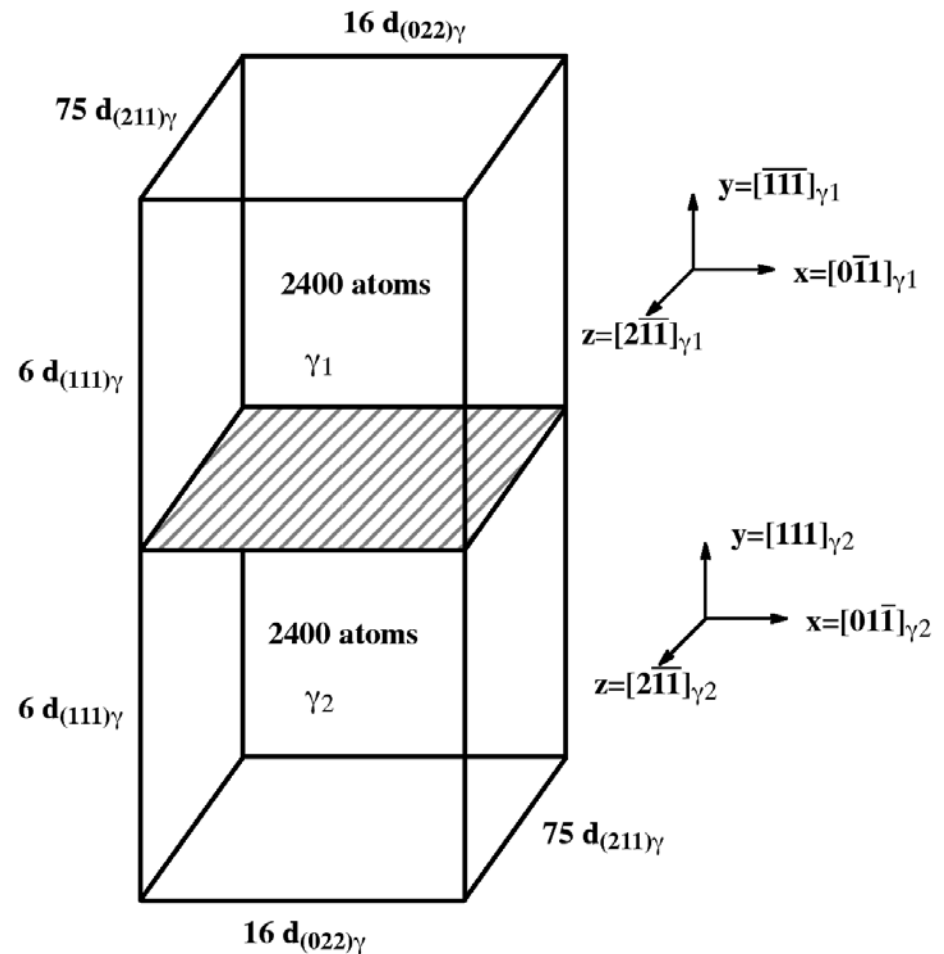
$$h^{\alpha\beta}(t) = q^{\alpha\beta} \left| 1 - \frac{s^\beta(t)}{s_s} \right|^r \operatorname{sign} \left\{ 1 - \frac{s^\beta(t)}{s_s} \right\}$$

$$s^\alpha(\tau) = s^\alpha(t) + \sum_{\beta} h^{\alpha\beta}(t) |\Delta\gamma^\beta(t)|$$

**FE Modeling of
Deformation and Fracture
in Polycrystalline
 γ -TiAl + α_2 -Ti₃Al
Single Crystals**

**Cohesive-Zone
Formulation of
Colony-Boundary and
Lamellar-Interface
Potentials**

Schematic:
 γ -TiAl/ γ -TiAl
 (γ_1/γ_2) bicrystal used
 for determination of
 the $(111)_{\gamma_1}/(111)_{\gamma_2}$
 lamellar interfacial
 potential.



Equilibrium Configuration:

$$[\bar{1}\bar{1}\bar{1}]_{\gamma_1} // [111]_{\gamma_2}$$

Lamellar Interface

Projections

(a) The

$$[01\bar{1}]_{\gamma_1} // [0\bar{1}1]_{\gamma_2}$$

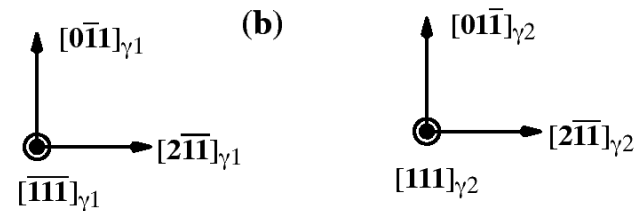
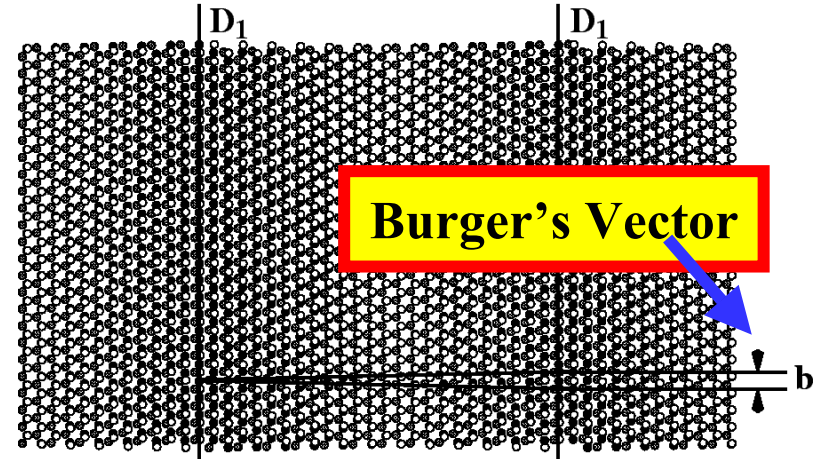
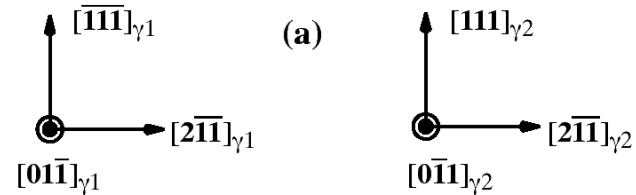
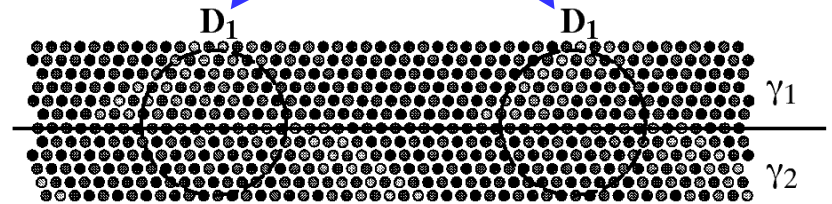
plane

(b) The

$$[\bar{1}\bar{1}\bar{1}]_{\gamma_1} // [111]_{\gamma_2}$$

plane

Dislocations



Variation of Interface Potential for

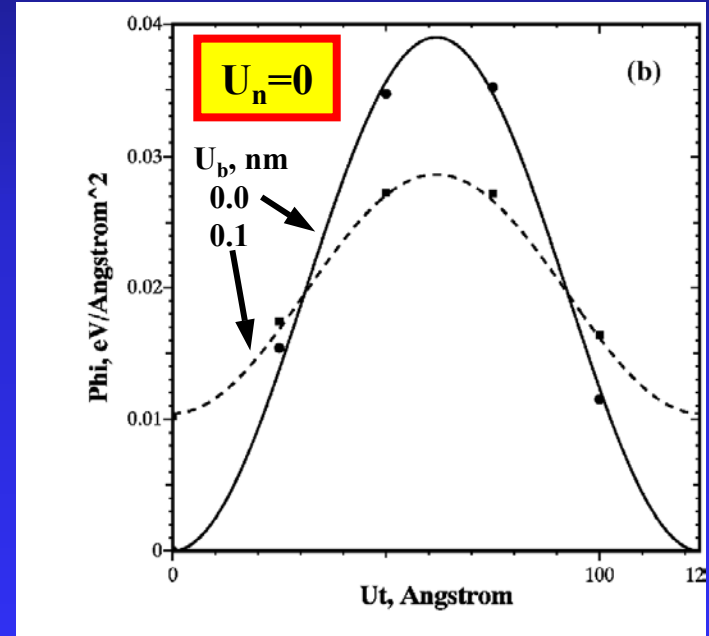
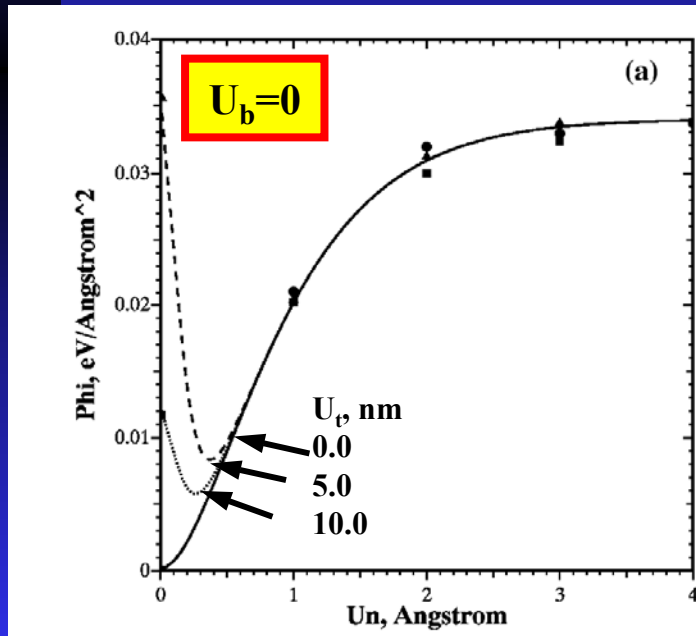
$$[\bar{1}\bar{1}\bar{1}]_{\gamma_1} // [111]_{\gamma_2}$$

Lamellar Interface

$$U_n \text{ along } [\bar{1}\bar{1}\bar{1}]_{\gamma_1} // [111]_{\gamma_2}$$

$$U_t \text{ along } [01\bar{1}]_{\gamma_1} // [0\bar{1}1]_{\gamma_2}$$

$$U_b \text{ along } [2\bar{1}\bar{1}]_{\gamma_1} // [2\bar{1}\bar{1}]_{\gamma_2}$$



**Relationship Between Interface Potential Function Φ
and U_n , U_t , and U_b for all γ -TiAl/ γ -TiAl Lamellar
Interfaces and Colony Boundaries Analyzed**

$$\Phi = \sigma_{\max} \delta_n \left[e - \left(\frac{U_n}{\delta_n} + 1 \right) \exp^{[(U_n/\delta_n)+1]} \right]$$

$$+ \frac{1}{2} \alpha_0 \left(\frac{6U_n}{\delta_n} + 1 \right) \exp^{(6U_n/\delta_n)}$$

$$\left\{ \alpha_1 + \left[\alpha_2 \sin \frac{4\pi(U_s - 2)}{\lambda_s} + \cos \left(\frac{2\pi U_s}{\lambda_s} + \alpha_3 \right) + \alpha_4 \right] \left(\alpha_5 + \cos \frac{2\pi U_b}{\lambda_b} \right) \right\}$$

Decohesion Potential Parameters for one γ -TiAl/ γ -TiAl Lamellar Interface and one colony boundary

Parameter	Interface Type	
	$(111)_{\gamma_1} / (111)_{\gamma_2}$ Lamellar Boundary	$(001)_{\gamma_1} / (0\bar{1}1)_{\gamma_2}$ Lamellar Boundary
n-Direction	$[\bar{1}\bar{1}\bar{1}]_{\gamma_1} / [111]_{\gamma_2}$	$[001]_{\gamma_1} / [0\bar{1}1]_{\gamma_2}$
t-Direction	$[\bar{1}\bar{1}\bar{1}]_{\gamma_1} / [111]_{\gamma_2}$	$[\bar{1}\bar{1}0]_{\gamma_1} / [\bar{1}\bar{1}\bar{1}]_{\gamma_2}$
b-Direction	$[\bar{1}\bar{1}\bar{1}]_{\gamma_1} / [111]_{\gamma_2}$	$[\bar{1}\bar{1}0]_{\gamma_1} / [2\bar{1}\bar{1}]_{\gamma_2}$
δ_n , nm	0.05	0.05
λ_t , nm	12.35	3.67
λ_b , nm	0.578	1.07

Table Cont'd ↓

Table Cont'd ↑

α_1	-0.039	-0.145
α_2	-1	0.42
α_3	0	-0.31
α_4	0	-3.42
α_5	0	1.17
α_0	0	-5.02
σ_{\max} , GPa	2.01	1.21
$\tau_{\max,t}$, GPa	0.160	12.7
$\tau_{\max,b}$, GPa	1.65	0.73
$\Phi(U_n \rightarrow \infty)$, J/m ²	0.561	0.374

Interface Elements

Reference Configuration

Nodes: $1=4$ & $2=3$

Internal Nodes

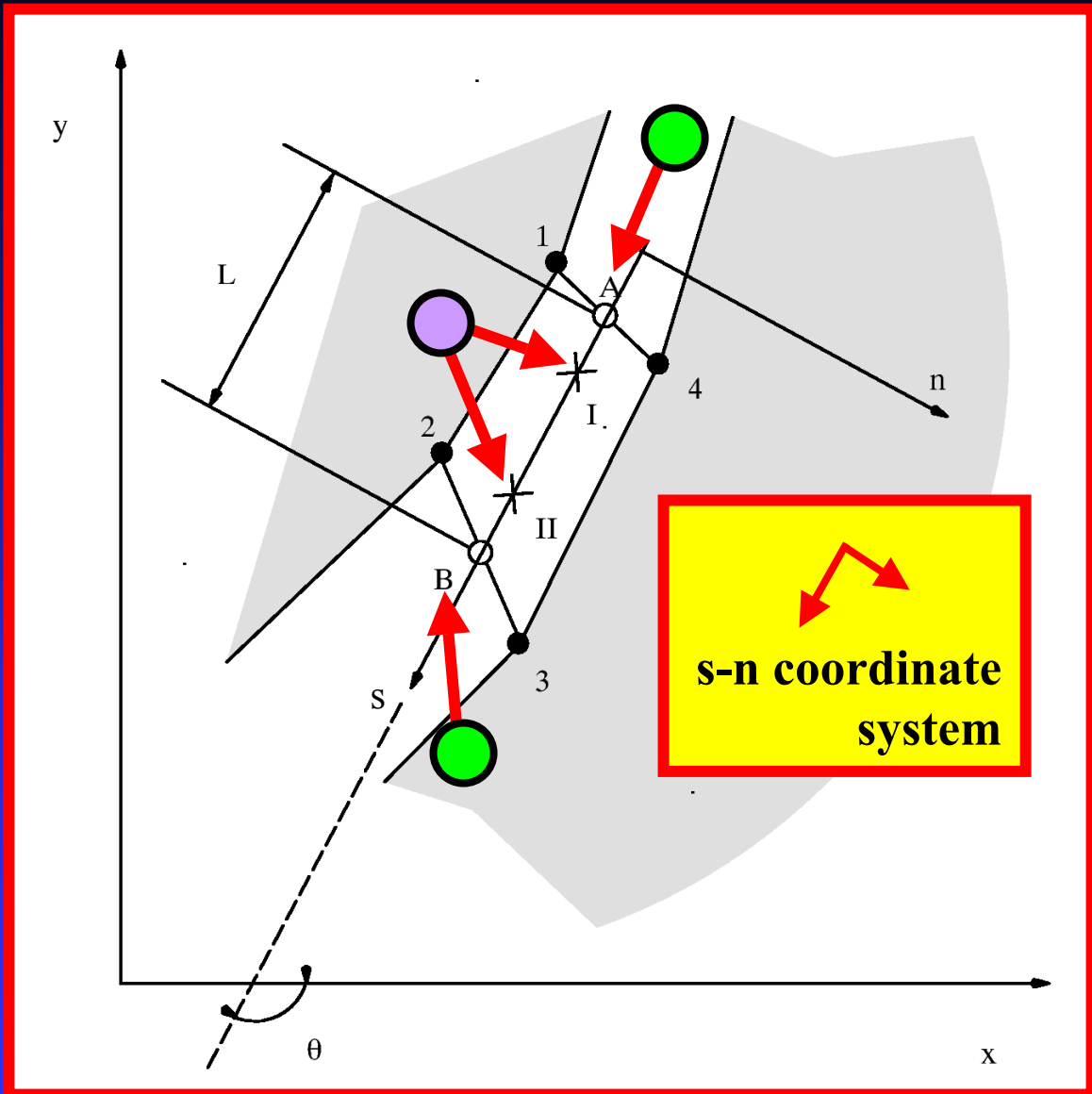


Nodes

Internal Nodes



Nodes



Interface Element Formulation

Interface Displacements:

Displacements at nodes A&B
mapped to those at nodes 1, 2, 3 and 4

$$U_n^A = (U_y^4 - U_y^1) \cos \theta - (U_x^4 - U_x^1) \sin \theta$$

$$U_s^A = (U_y^4 - U_y^1) \sin \theta - (U_x^4 - U_x^1) \cos \theta$$

$$U_n^B = (U_y^3 - U_y^2) \cos \theta - (U_x^3 - U_x^2) \sin \theta$$

$$U_n^A = (U_y^4 - U_y^1) \cos \theta - (U_x^4 - U_x^1) \sin \theta$$

Interface Element Formulation

Cont'd:

Normal and Tangential Components of Interface Displacements:

$$U_s(\eta) = N_A(\eta)U_s^A + N_B(\eta)U_s^B$$

$$U_n(\eta) = N_A(\eta)U_n^A + N_B(\eta)U_n^B$$

Virtual Work Equation:

$$\int_{-1}^1 \delta\Phi(\eta) L \pi r(\eta) d\eta = \sum_{I=n,s} \sum_{N=A,B} F_I^N \delta U_I^N$$

Interface Element Formulation

Cont'd:

Perturbation of Interface Potential:

$$\begin{aligned} \delta\Phi = & \frac{\partial\Phi[U_s(\eta), U_n(\eta)]}{\partial U_n} [N_A(\eta)\delta U_n^A + N_B(\eta)\delta U_n^B] \\ & + \frac{\partial\Phi[U_s(\eta), U_n(\eta)]}{\partial U_s} [N_A(\eta)\delta U_s^A + N_B(\eta)\delta U_s^B] \end{aligned}$$

Force Components at Nodes A and B:

$$F_I^N = \int_{-1}^1 \frac{\partial\Phi[U_s(\eta), U_n(\eta)]}{\partial U_I} N_N(\eta) L \pi r(\eta) d\eta$$

Interface Element Formulation

Cont'd:

Residual Nodal Forces in Global Coordinate System:

$$\begin{aligned}R_x^1 &= -R_x^4 = F_s^A \cos \theta - F_n^A \sin \theta \\R_y^1 &= -R_y^4 = F_s^A \sin \theta - F_n^A \cos \theta \\R_x^2 &= -R_x^3 = F_s^B \cos \theta - F_n^B \sin \theta \\R_y^2 &= -R_y^3 = F_s^B \sin \theta - F_n^B \cos \theta\end{aligned}$$

Components of the Element jacobian:

$$\frac{\partial R_j^i}{\partial U_I^k} = \sum_{I=n.s} \sum_{N=A.B} \sum_{j=n.s} \sum_{M=A.B} \frac{\partial R_j^i}{\partial F_I^N} \frac{\partial F_I^N}{\partial U_J^M} \frac{\partial U_J^M}{\partial U_I^k}$$


Finite Element

Formulation and

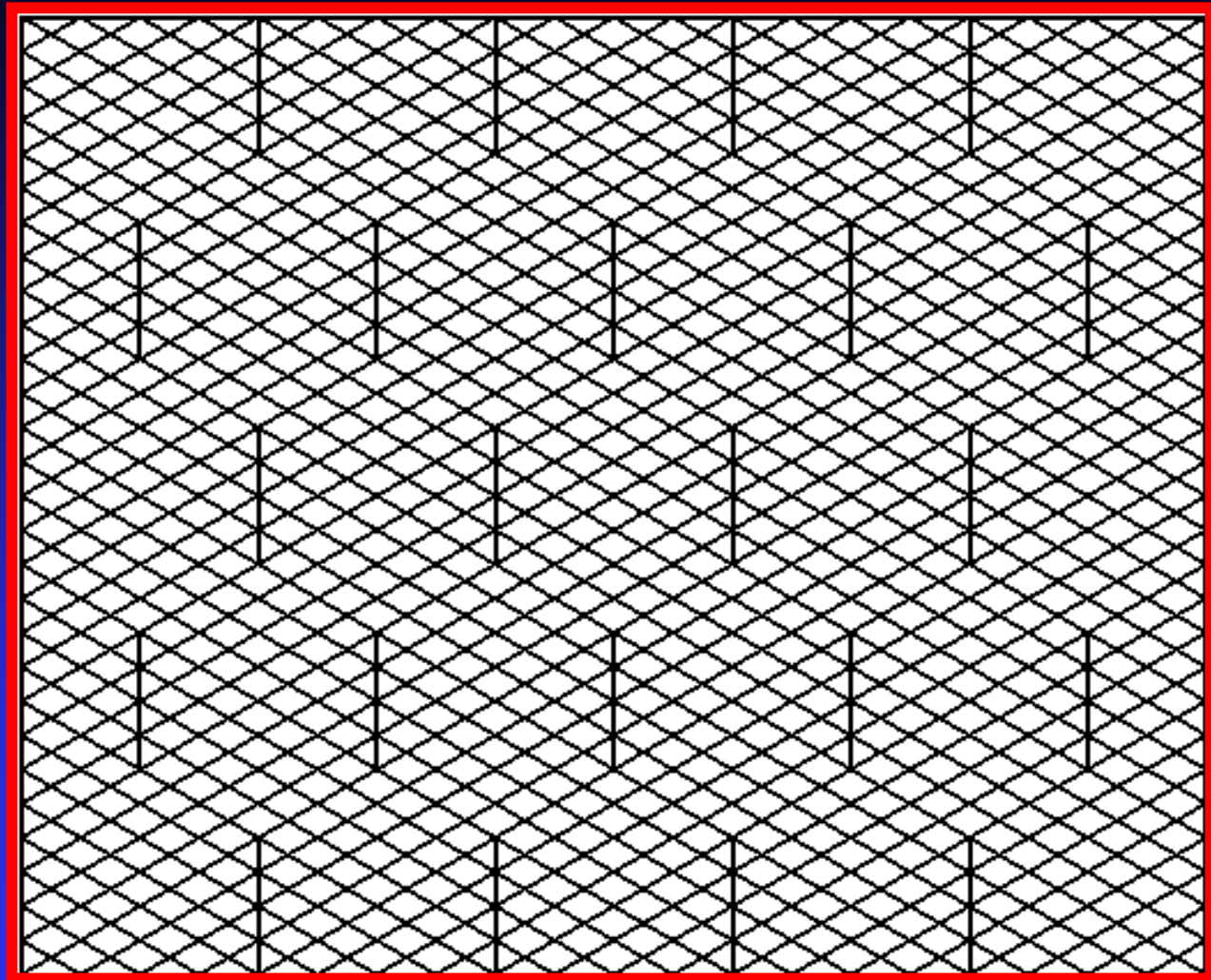
Results

Polycrystalline Aggregate

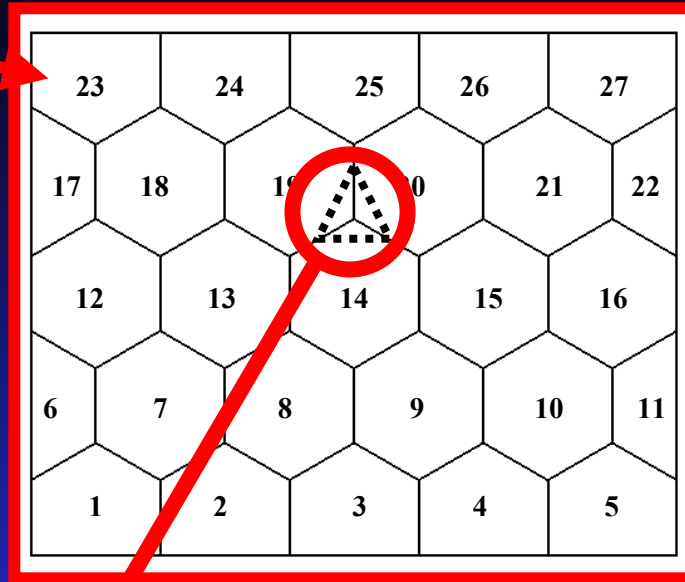
Finite Element Mesh

 → 971

 → 364

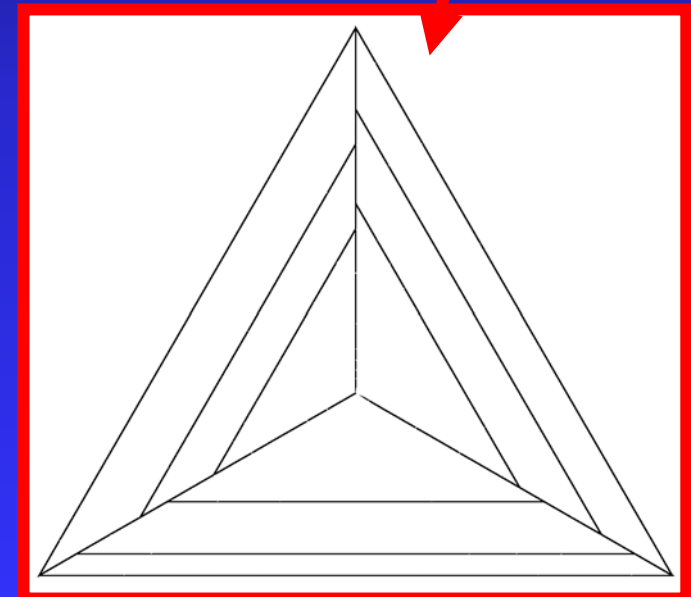
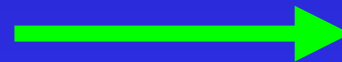
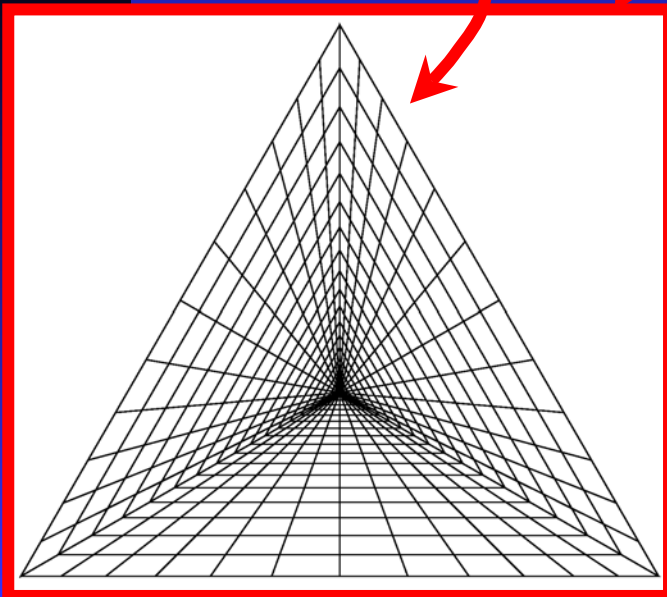
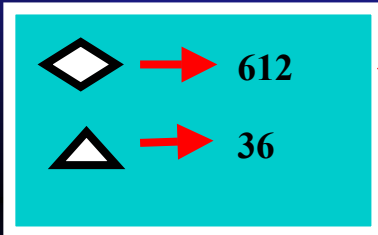


**Polycrystalline
Aggregate of
27 Lamellar
Colonies**



**Reference
Configuration
With 3 Lamellar
Colonies Each
Having 2 Lamellar
Boundaries**

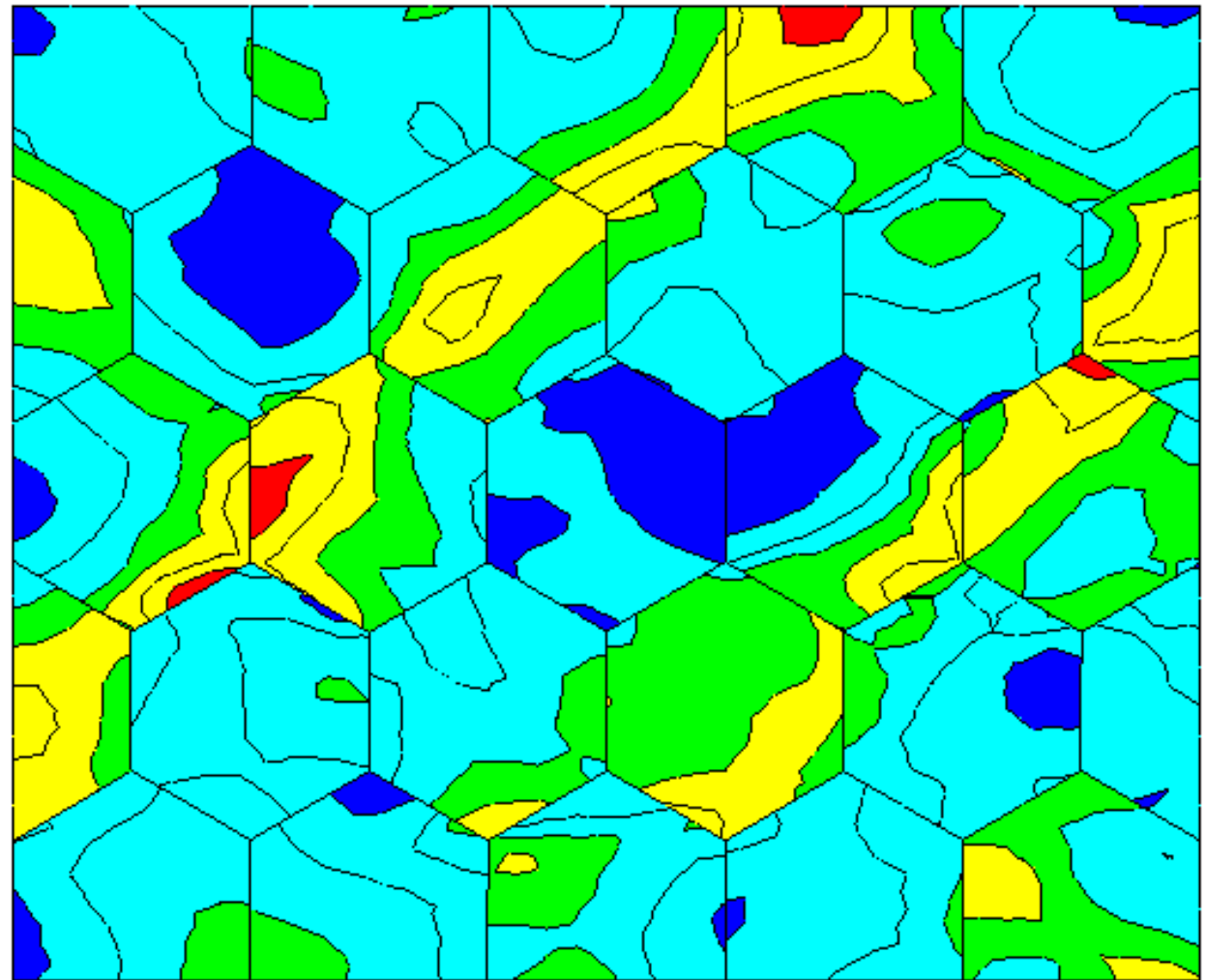
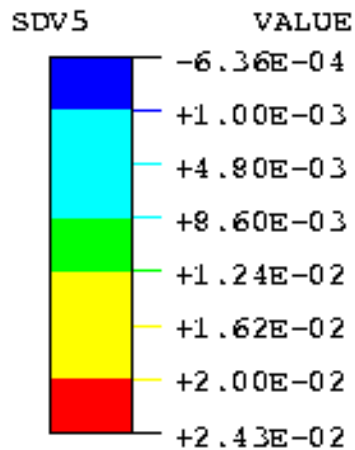
Finite Element Mesh



Results

Equivalent
Plastic
Strain

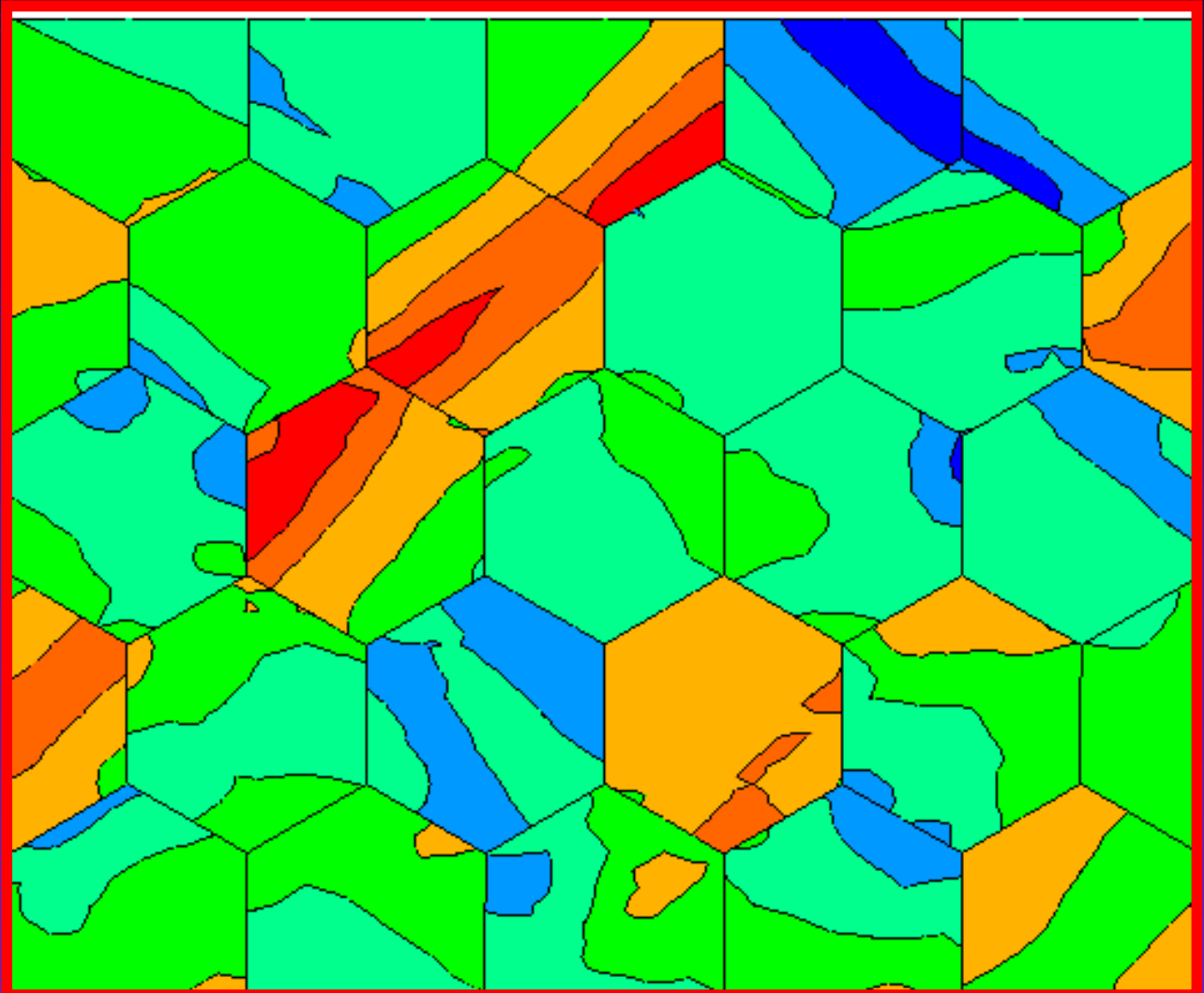
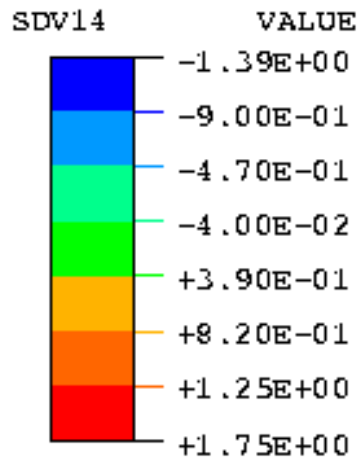
$\epsilon=0.015$



Results Contd.

Lattice
Rotation

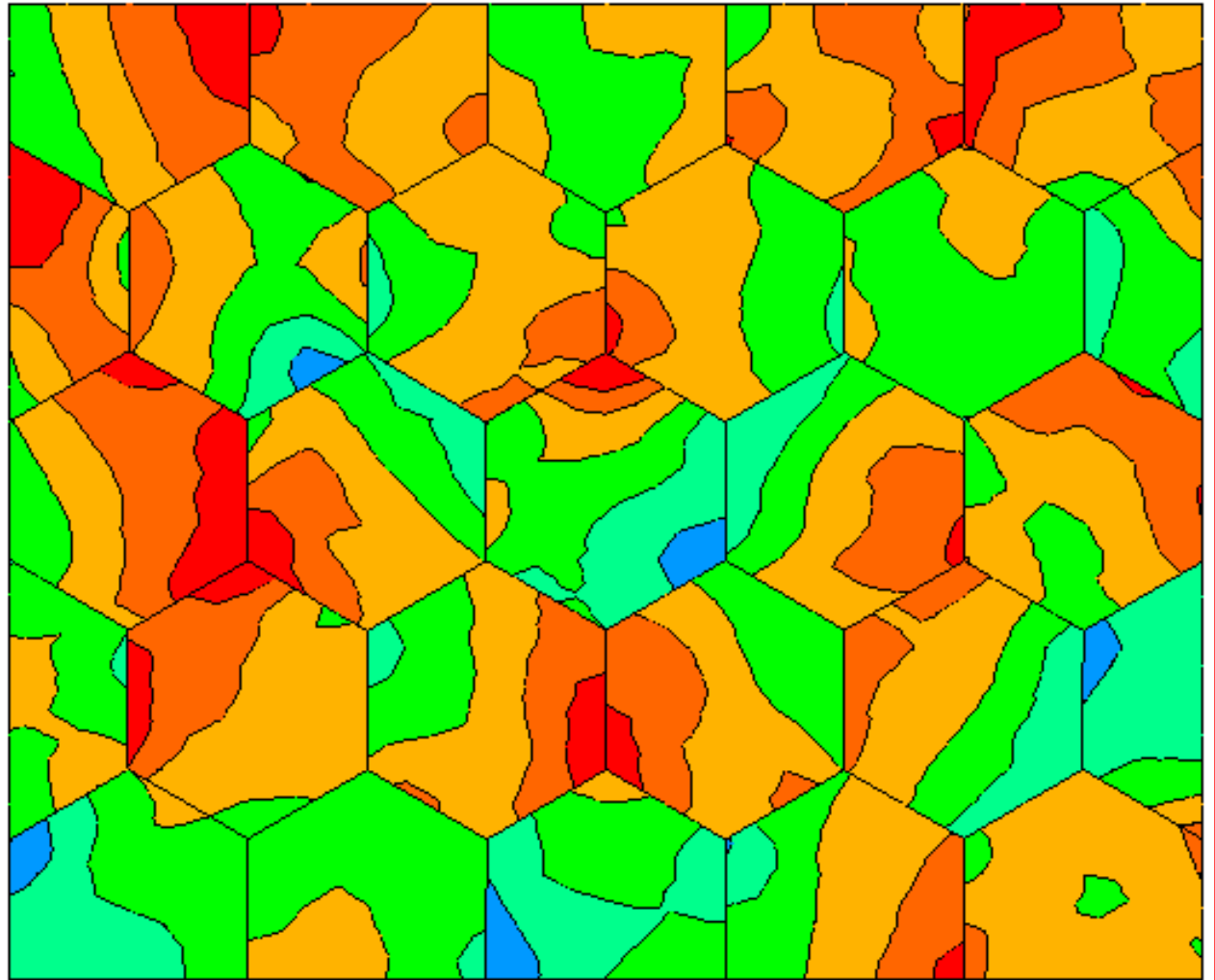
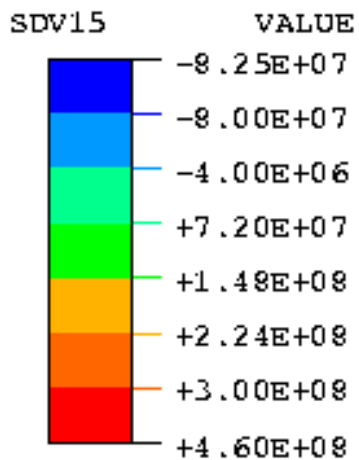
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Results Contd.

Hydrostatic
Stress

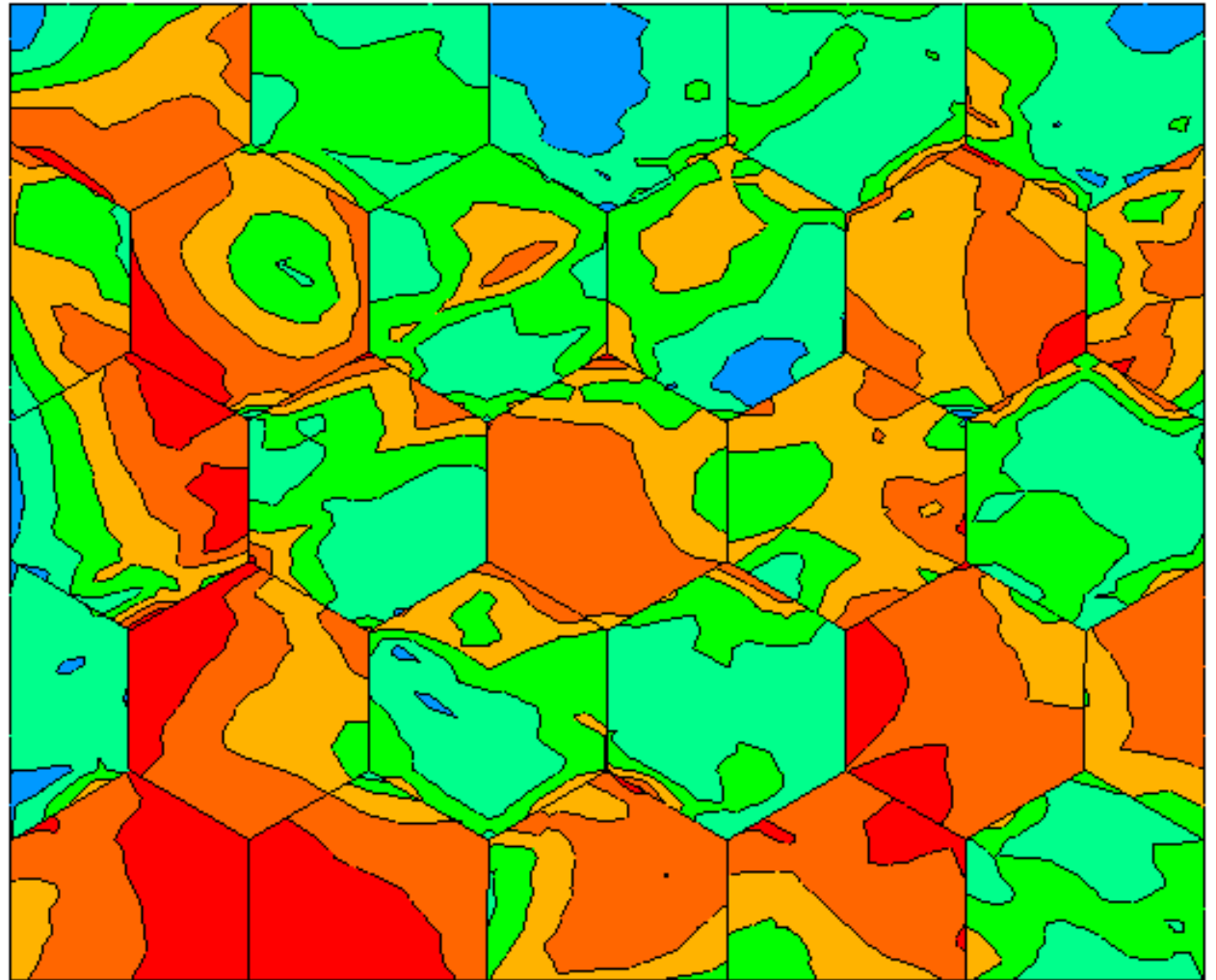
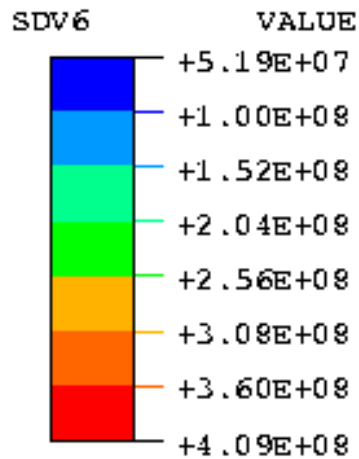
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Results Contd.

Equivalent
Stress

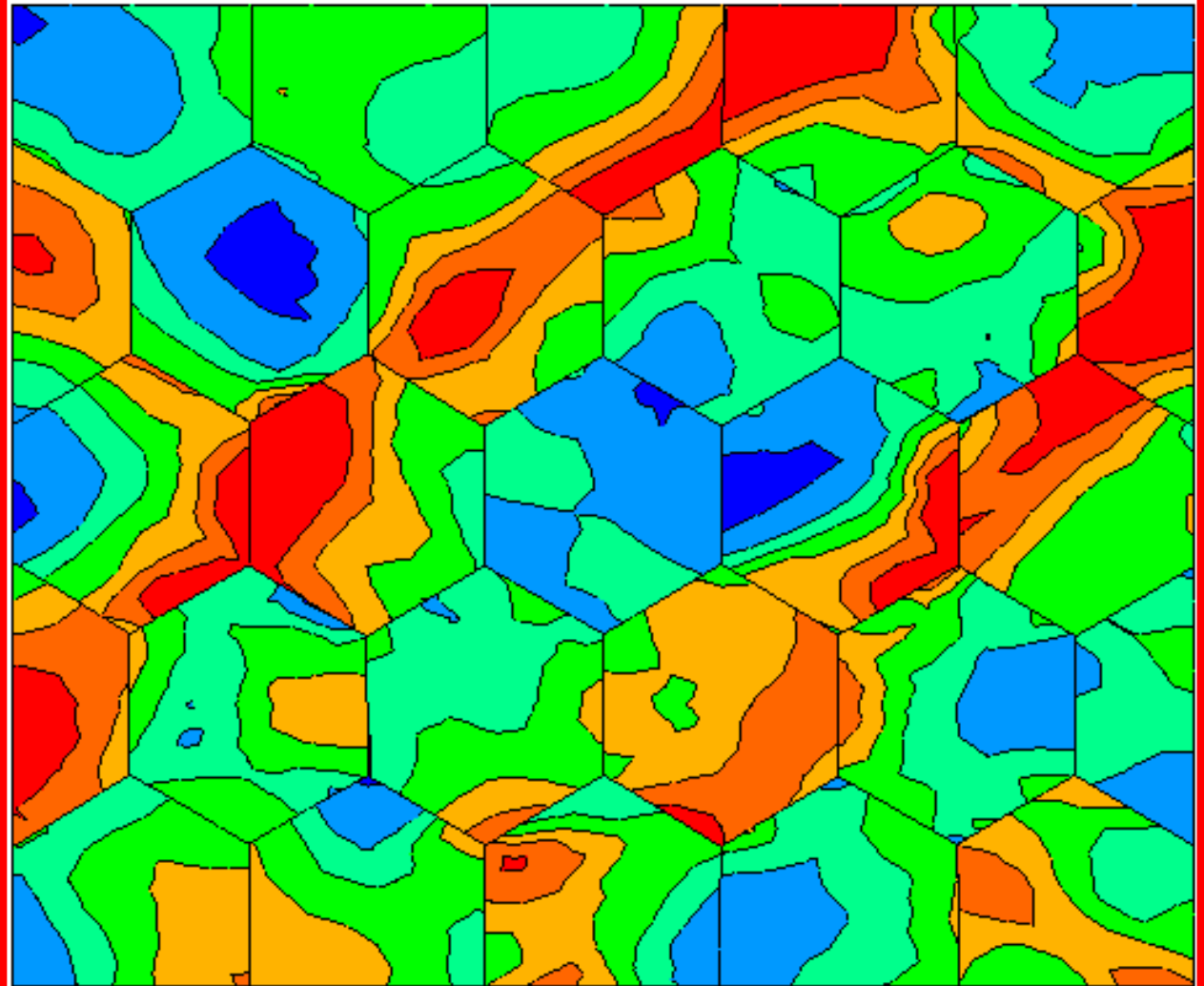
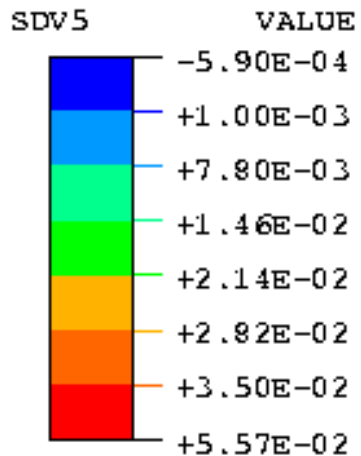
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Results Contd.

Equivalent
Plastic
Strain

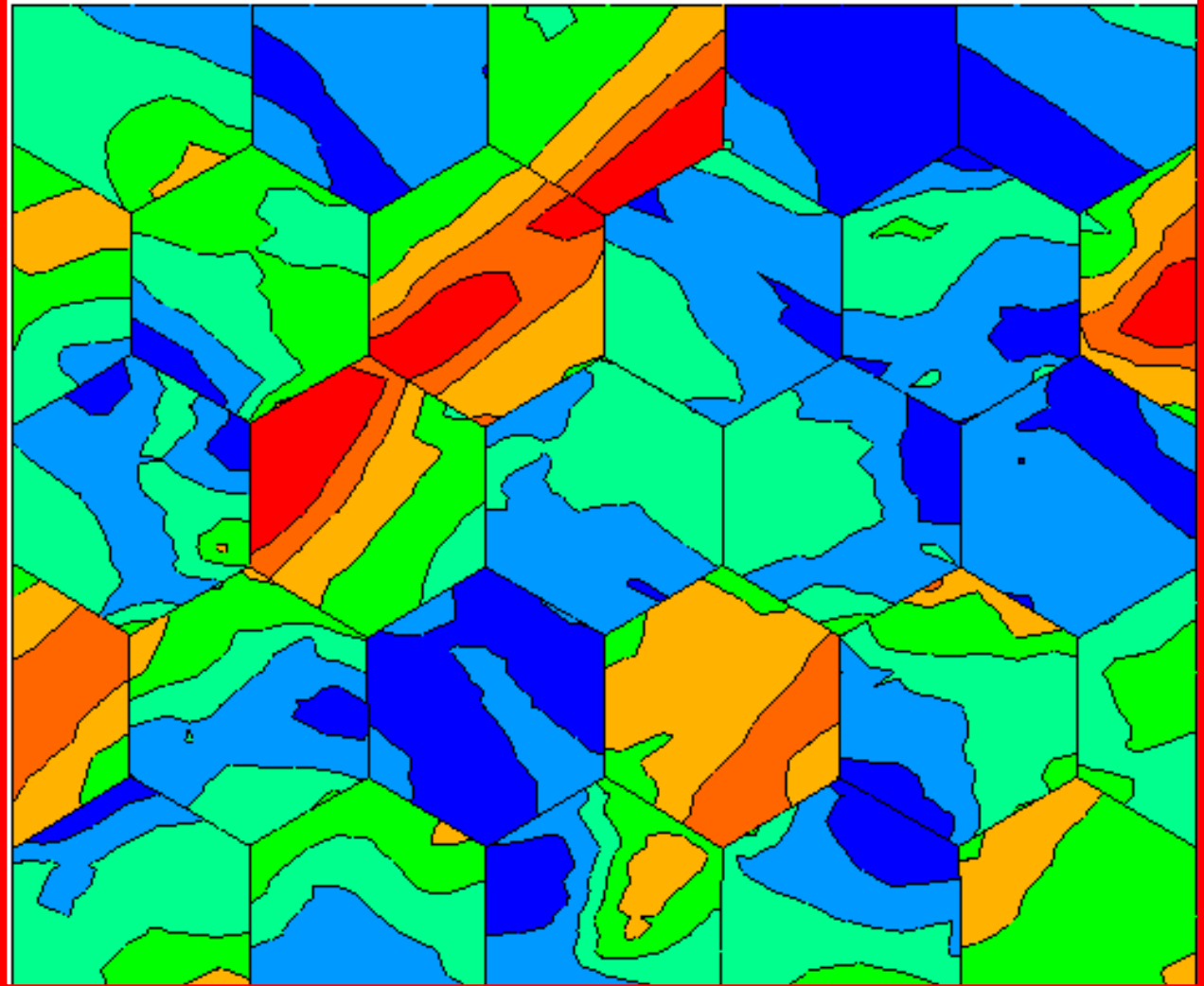
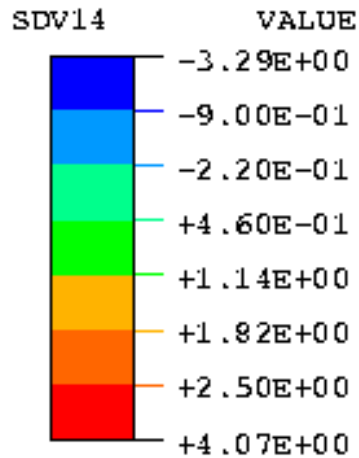
$$\epsilon = 0.03$$



Results Contd.

Lattice
Rotation

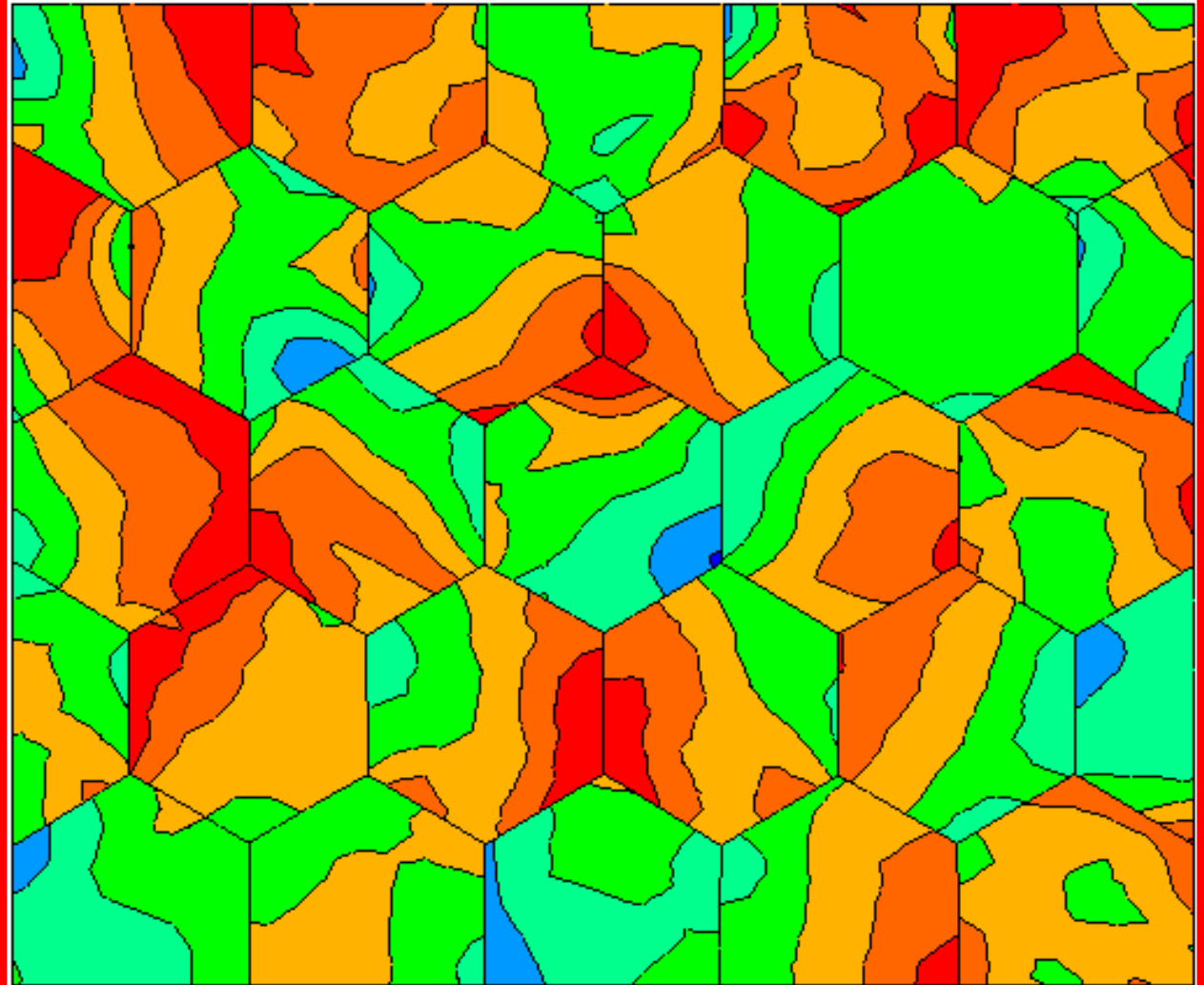
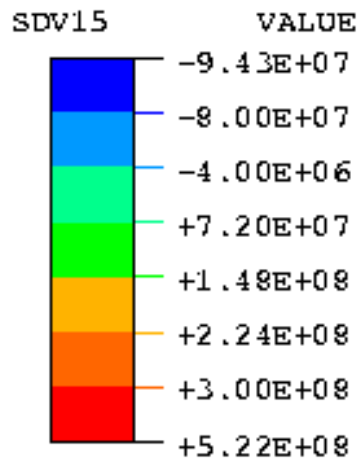
$\varepsilon=0.03$



Results Contd.

Hydrostatic
Stress

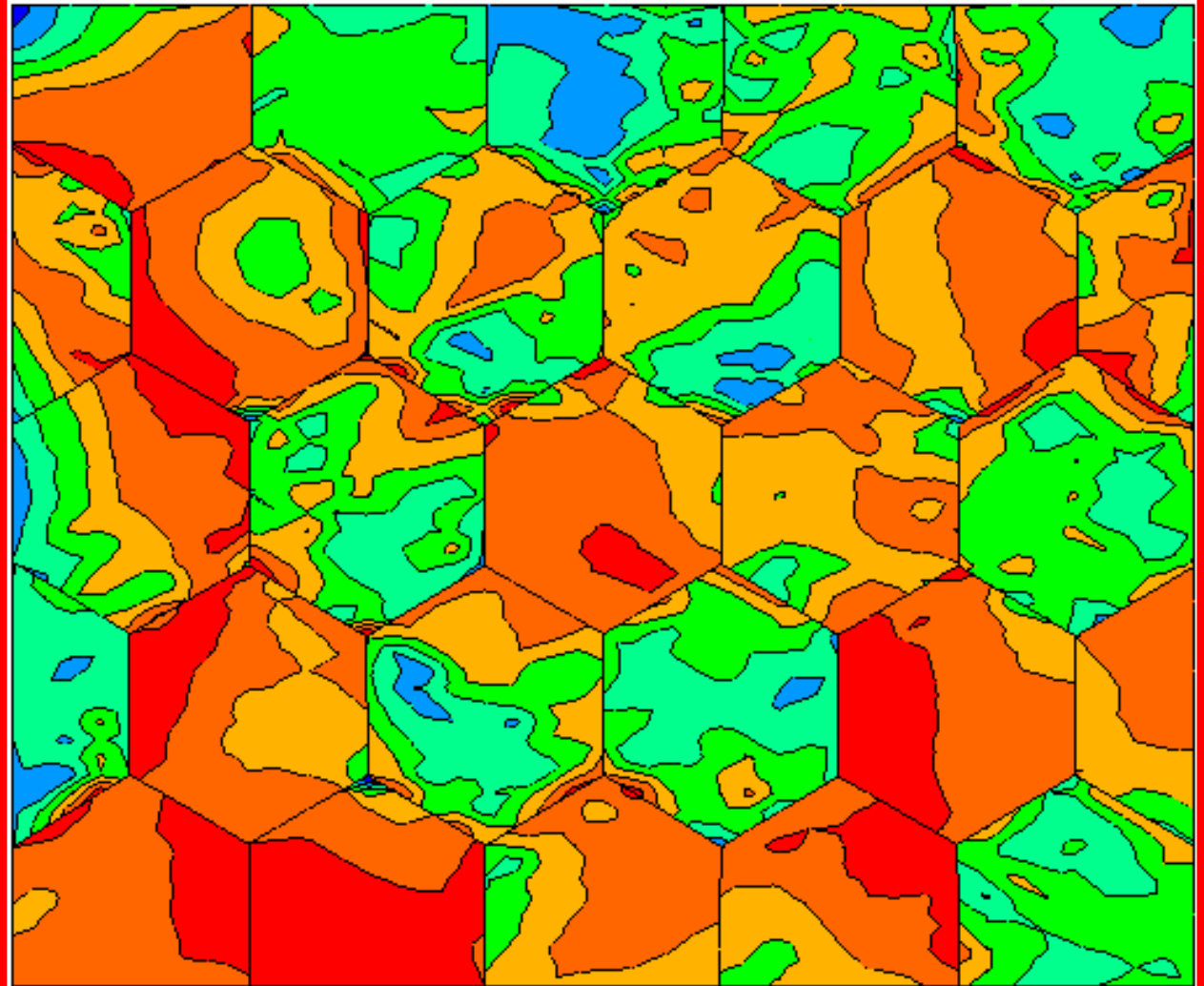
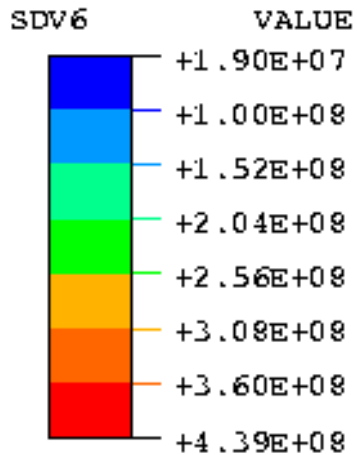
$\varepsilon=0.03$



Results Contd.

Equivalent
Stress

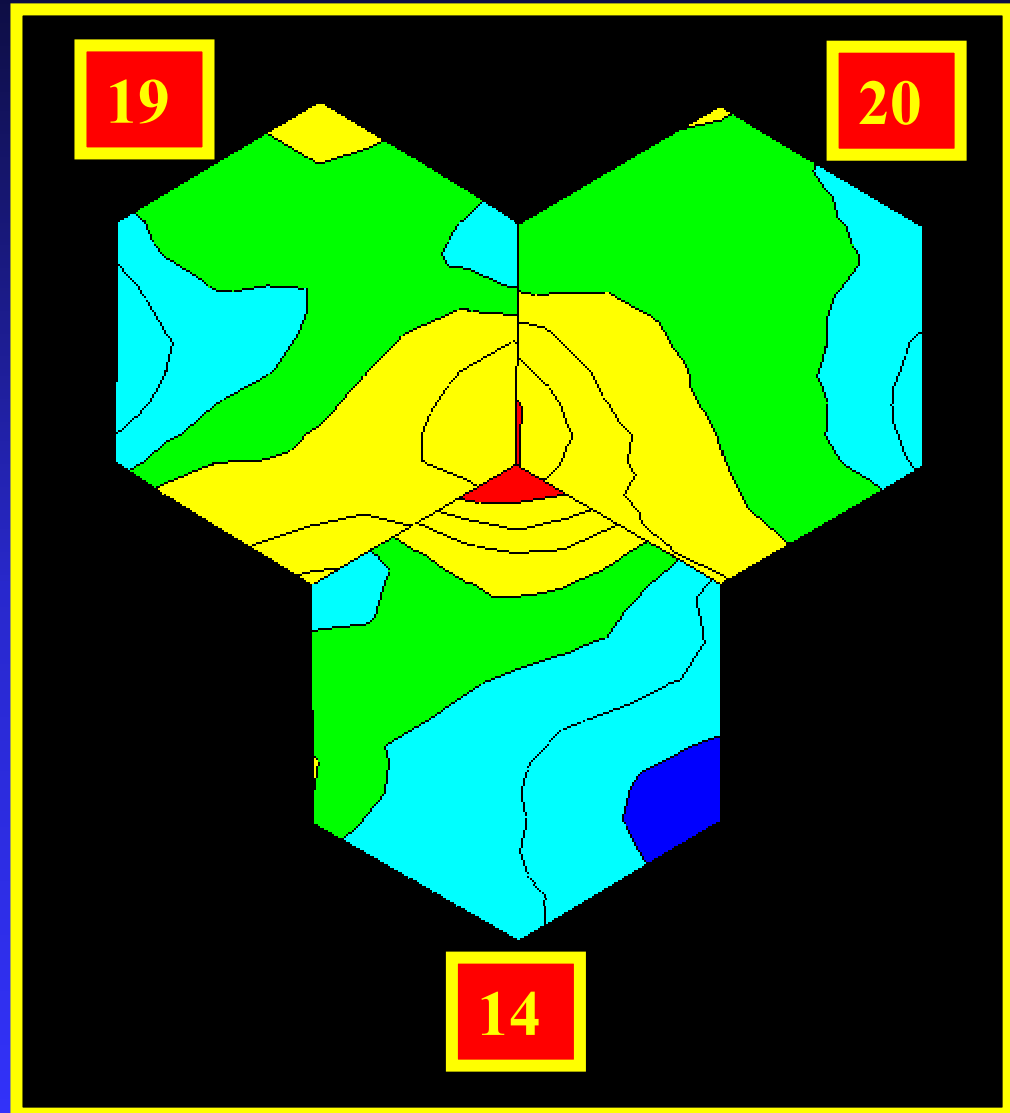
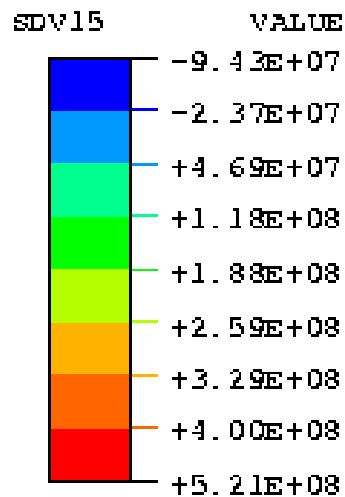
$$\varepsilon=0.03$$



Results Contd.

Hydrostatic
Stress

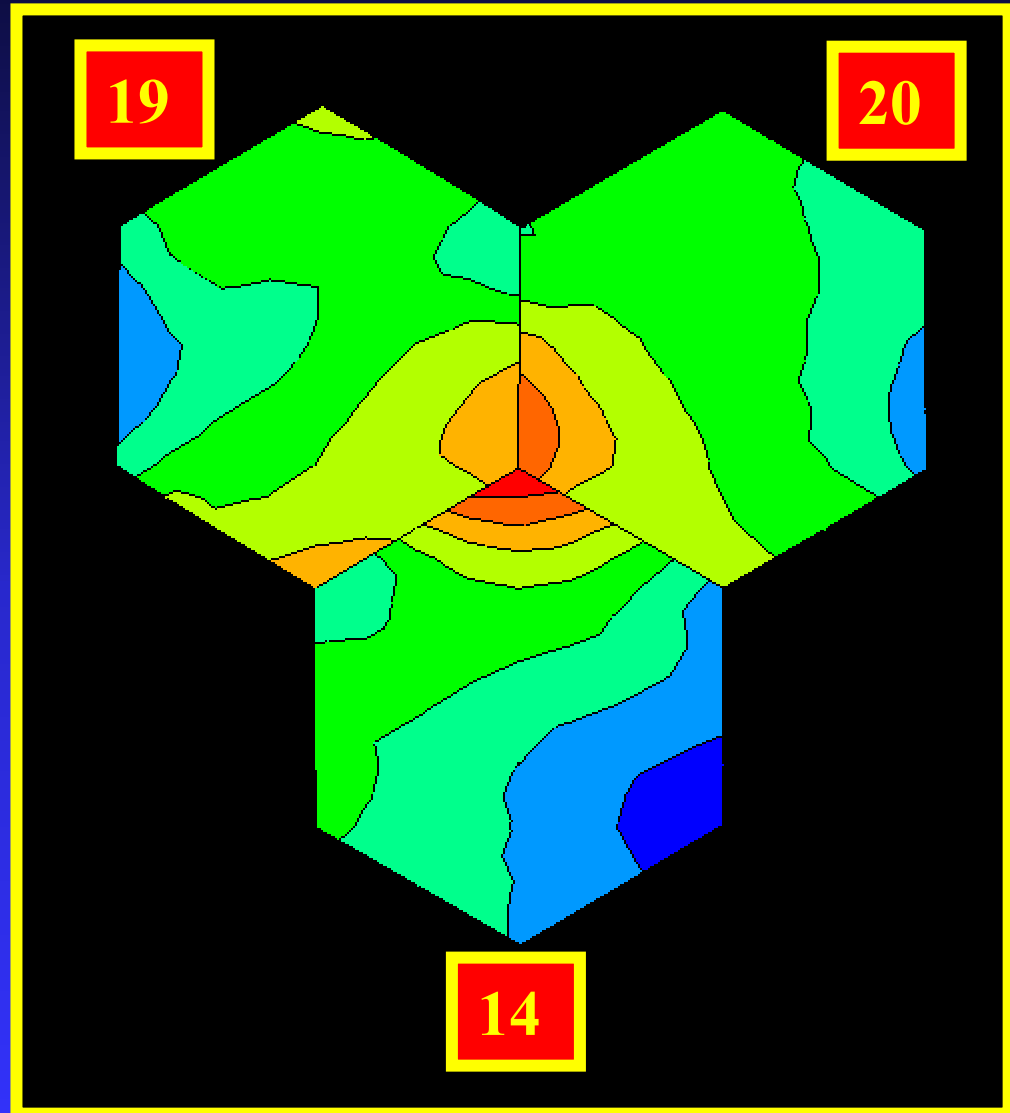
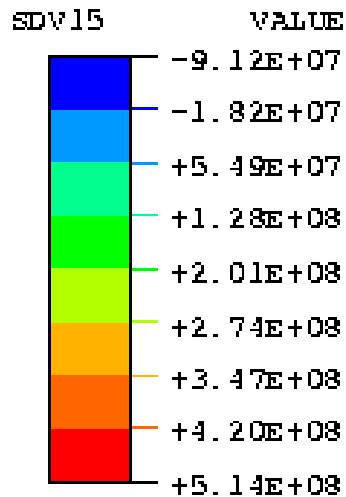
$\varepsilon=0.03$



Results Contd.

Hydrostatic
Stress

$\varepsilon=0.0319$



Results Contd.

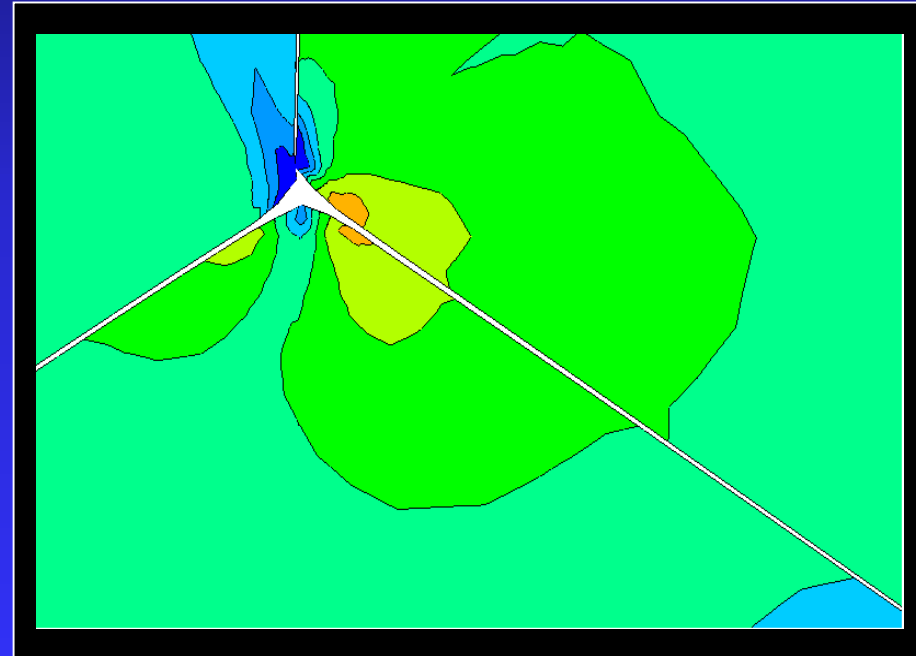
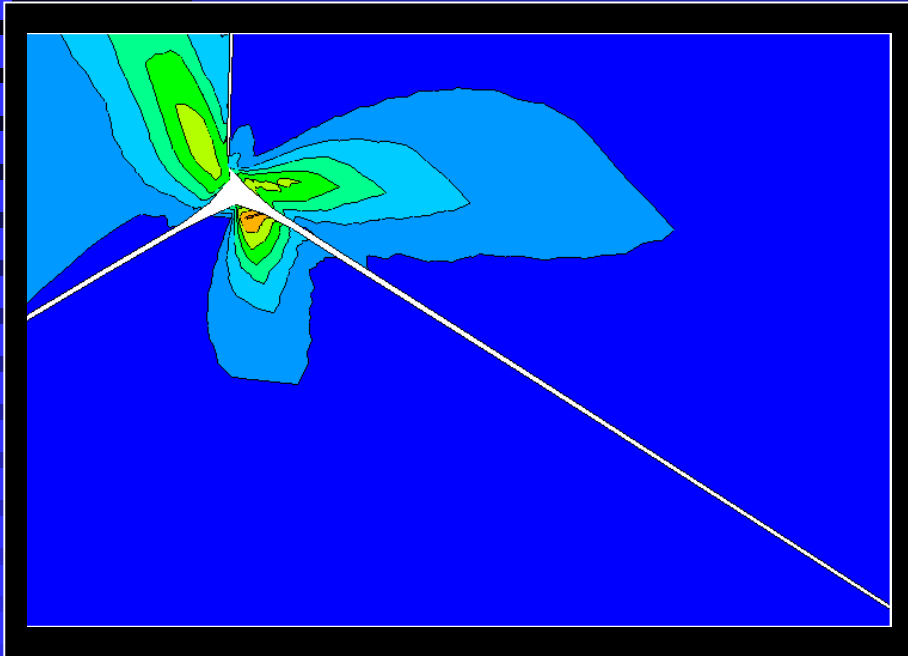
**Around 3-Colony
Junction**

$\varepsilon=0.025$

**No Lamellar
Interfaces**

Equivalent Plastic Strain

Hydrostatic Stress



Results Contd.

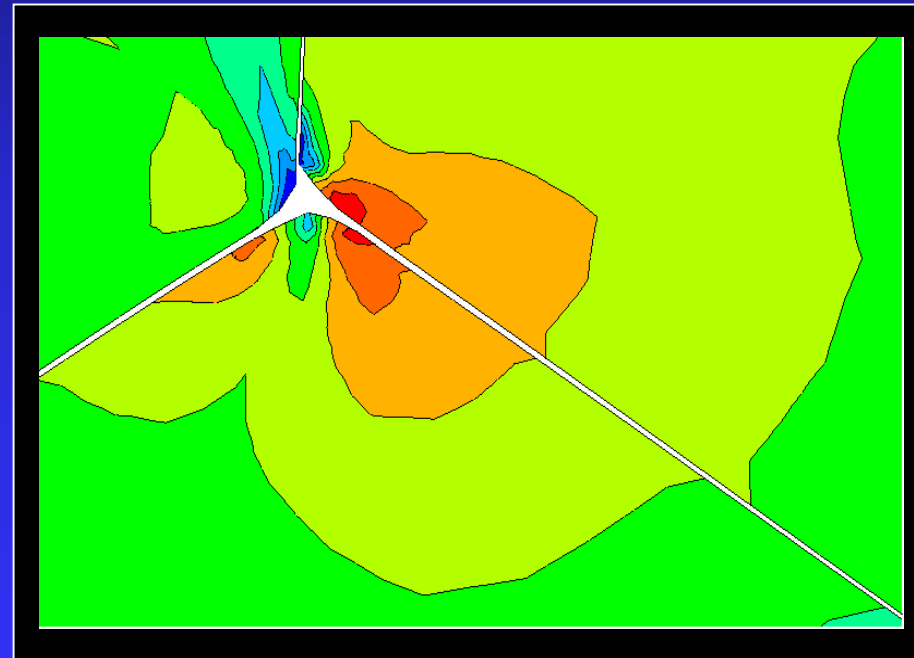
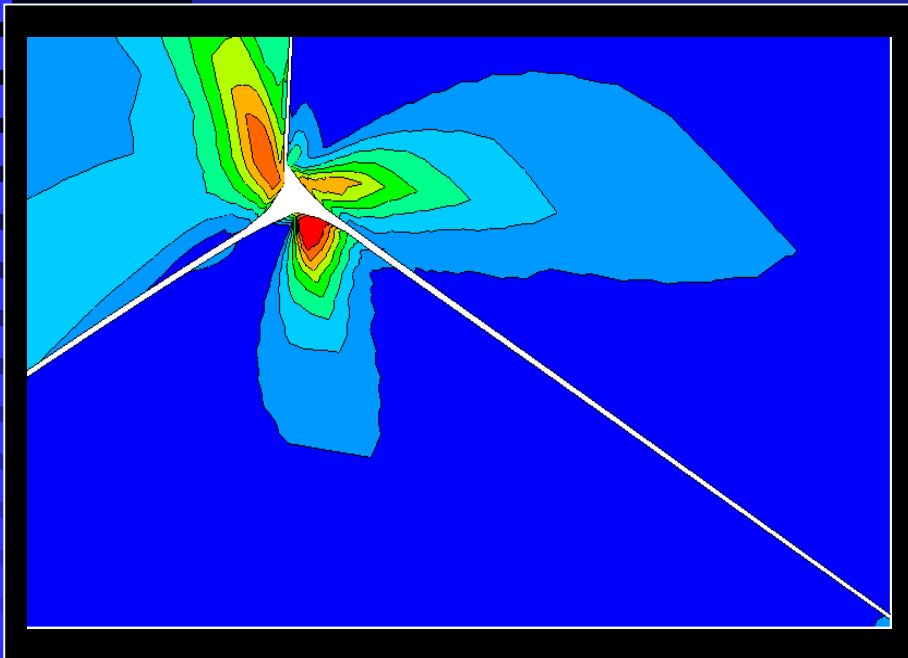
**Around 3-Colony
Junction**

$\varepsilon=0.030$

**No Lamellar
Interfaces**

Equivalent Plastic Strain

Hydrostatic Stress



Results Contd.

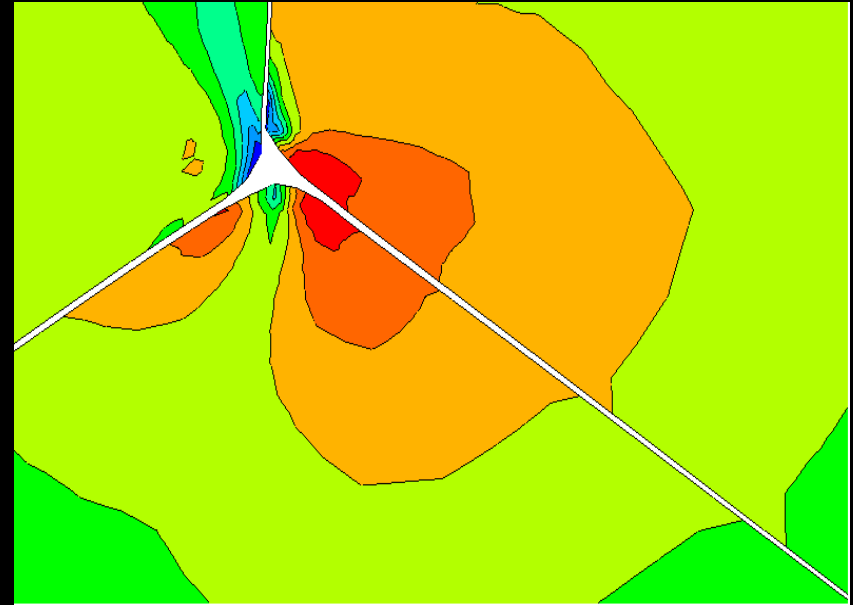
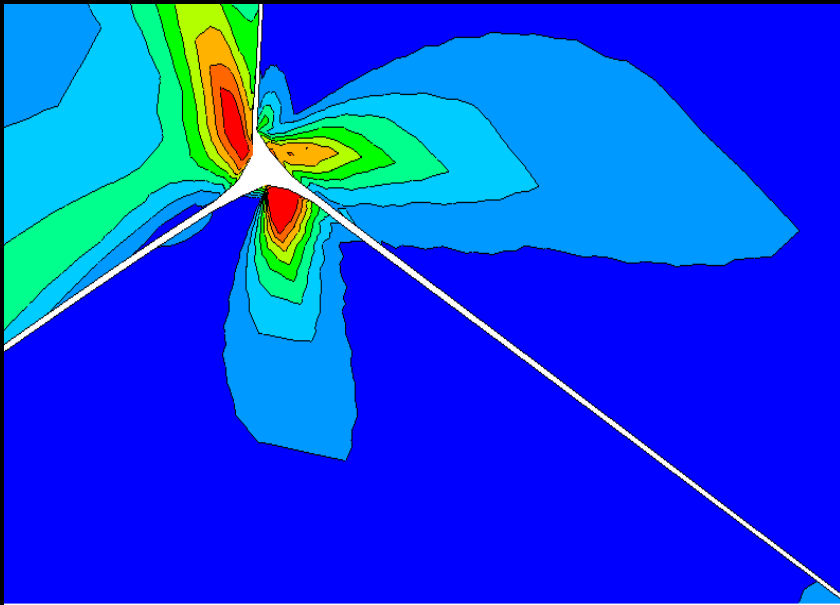
**Around 3-Colony
Junction**

$\varepsilon=0.0319$

**No Lamellar
Interfaces**

Equivalent Plastic Strain

Hydrostatic Stress



Results Contd.

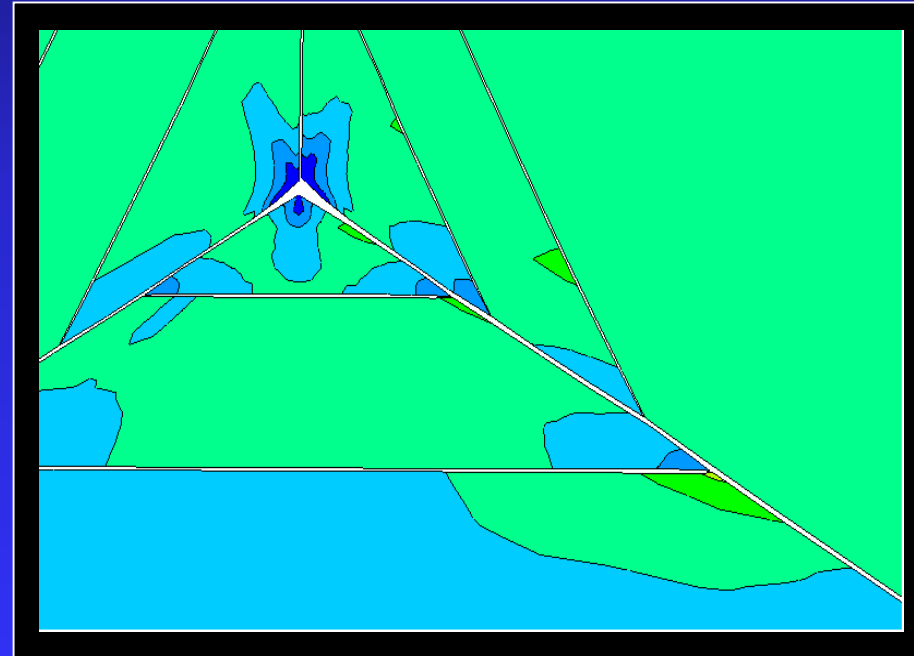
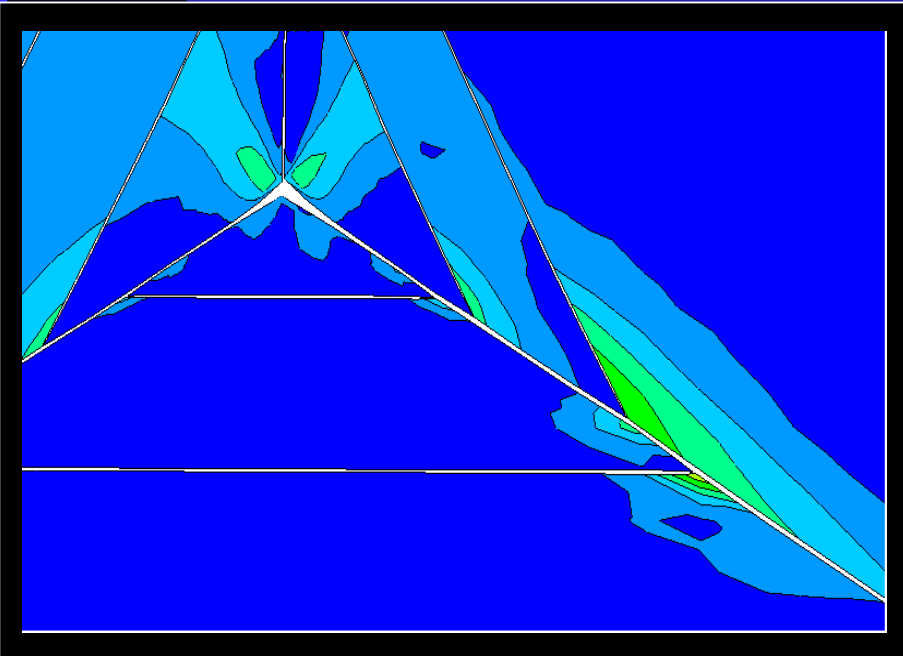
**Around 3-Colony
Junction**

$$\varepsilon=0.0250$$

**With Lamellar
Interfaces**

Equivalent Plastic Strain

Hydrostatic Stress



Results Contd.

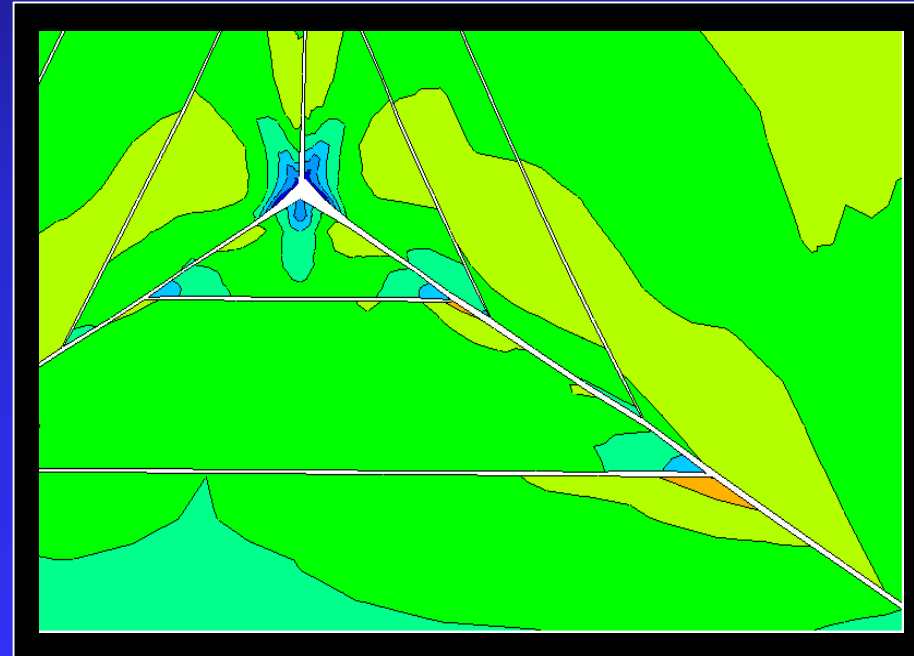
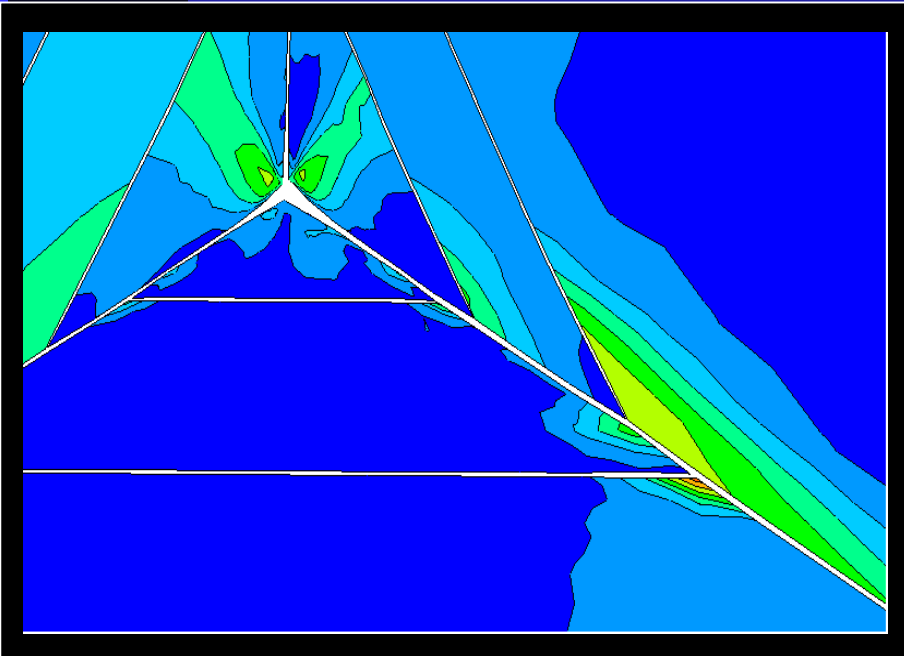
**Around 3-Colony
Junction**

$$\varepsilon=0.030$$

**With Lamellar
Interfaces**

Equivalent Plastic Strain

Hydrostatic Stress



Results Contd.

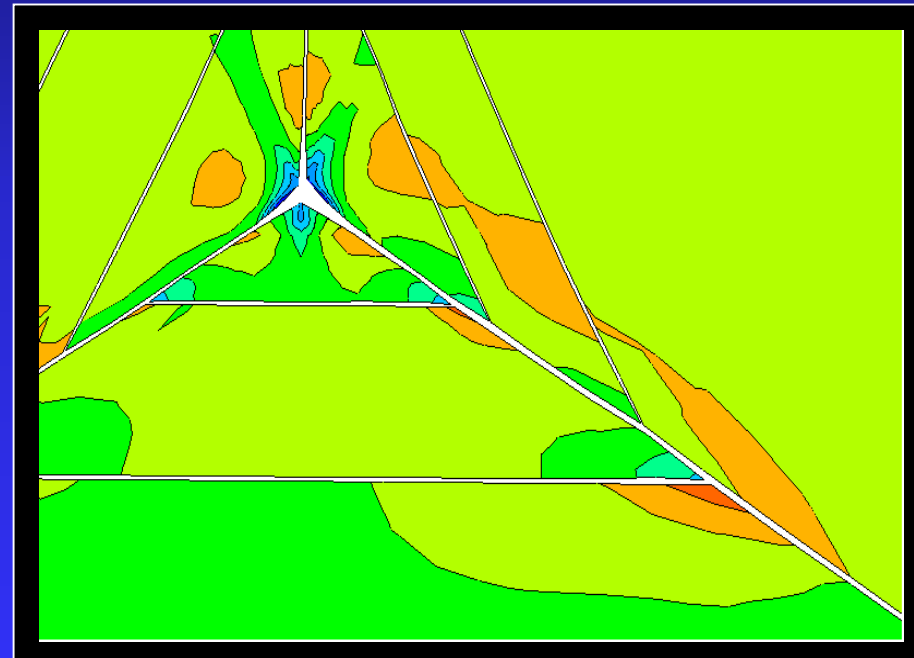
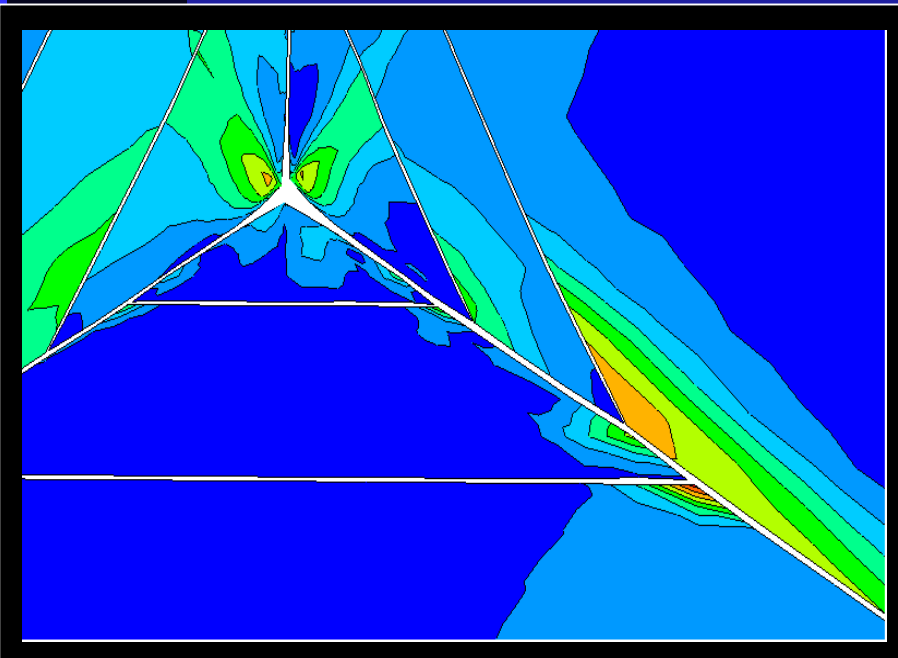
**Around 3-Colony
Junction**

$$\varepsilon=0.0319$$

**With Lamellar
Interfaces**

Equivalent Plastic Strain

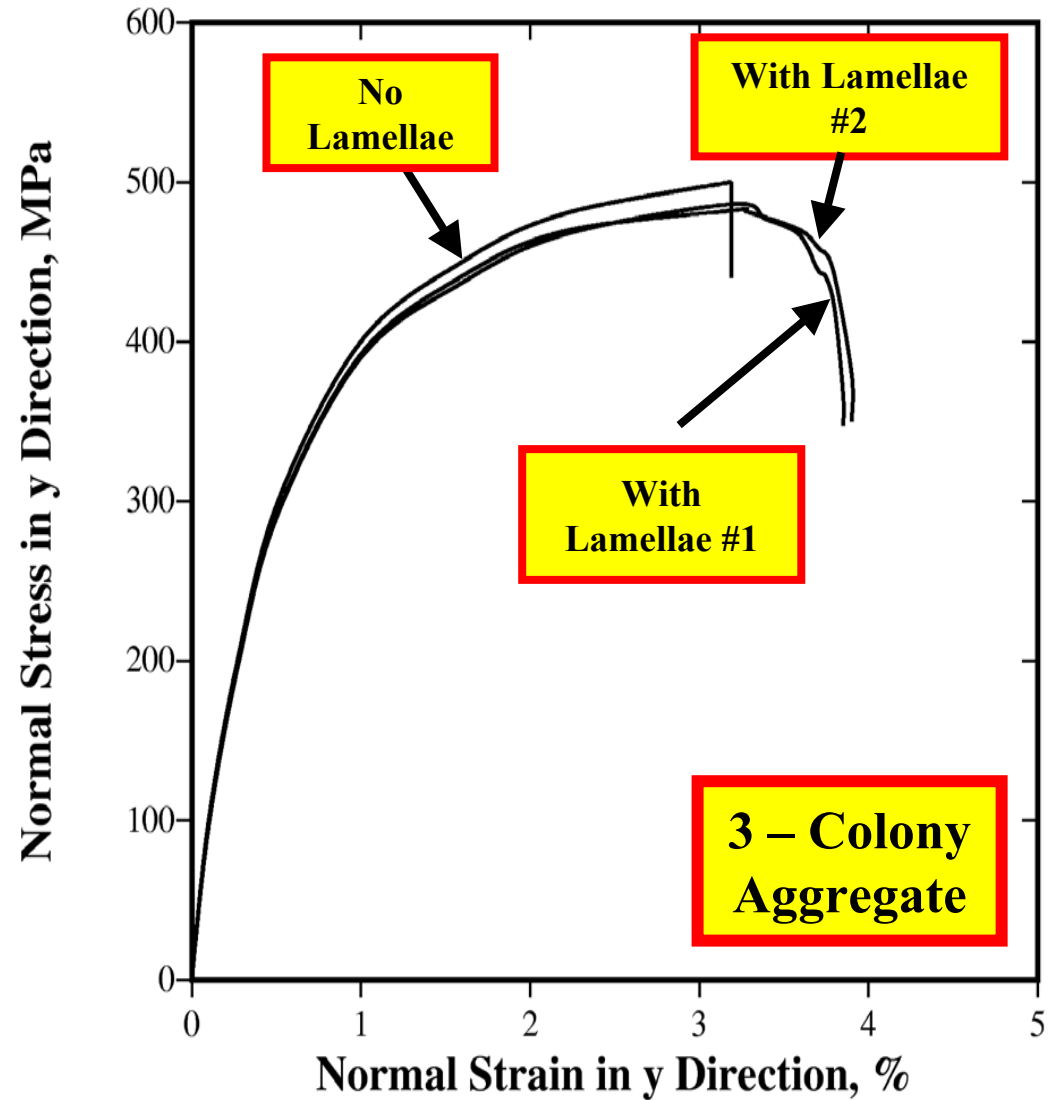
Hydrostatic Stress



Results Contd.

Normal Stress
Vs Normal
Strain

y-Direction



Conclusions

Conclusions

- **Crystal Plasticity can reasonably well account for deformation behavior of γ -TiAl and α_2 -Ti₃Al Single Crystals as well as γ -TiAl + α_2 -Ti₃Al Polysynthetically-Twinned Single Crystals.**
- **Deformation Behavior in Polysynthetically Twinned Single and Polycrystalline γ -TiAl + α_2 -Ti₃Al alloys is Dominated by Soft-Mode Slip in γ -TiAl and Hard-Mode Slip in α_2 -Ti₃Al.**
- **Plastic Flow Incompatibilities Near Some Three-Colony Junctions Gives Rise to Tensile Hydrostatic Stresses and Inter-Colony Fracture.**
- **Presence of Interlamellar Boundaries in Colonies Leads to Delocalization of Fracture and in Turn, to a Higher Damage Resistance of the Material.**
- **Good Agreement With Experiments Relative to the Role of lamellar and Colony Boundaries on Fracture Toughness and Initiation of Fracture.**

