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WORKING PARTY ON
MODELLING THERMOMECHANICAL BEHAVIOUR OF MATERIALS
(29 May - 16 June 1989)

POLYCRYSTAL PLASTICITY REVISITED AND PLASTIC DEFORMATION OF HEXAGONALS

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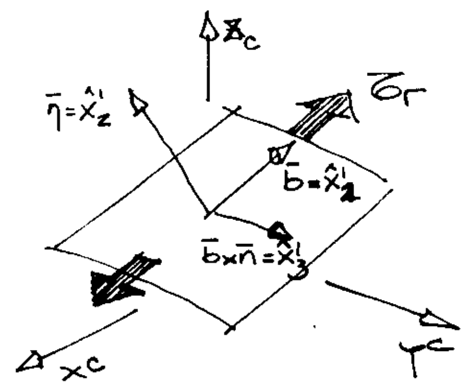
POLYCRYSTAL PLASTICITY REVISITED.

1- FLUX CHART OF TEXTURE DEVELOPMENT SIMULATION

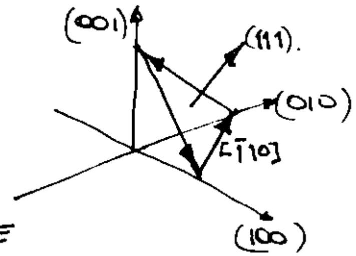
a) REPRESENT POLYCRYSTAL AS A DISCRETE COLLECTION OF GRAINS WITH INITIAL WEIGHTS	* INITIAL TEXTURE
b) IMPOSE INCREMENTAL DEFORMATION STEPS TO THE AGGREGATE. DERIVE $\Delta\varepsilon^g$, σ^g and $\Delta\gamma^g$ FOR EACH GRAIN.	* DEFORMATION MODEL. * CONSTITUTIVE LAW FOR THE GRAINS * ACTIVE SYSTEMS.
c) REORIENT EACH GRAIN BECAUSE OF SLIP & TWINNING.	* KINEMATICS * TWINNING MODEL. * ROTATION MATRICES.
d) REPEAT b) & c) UNTIL ACHIEVING FINAL DEFORMATION	* FINAL TEXTURE. * STATISTICS. * STRESS-STRAIN CURVE.
e) CALCULATE MECHANICAL RESPONSE OF TEXTURED MATERIAL.	



Slip system

$\bar\eta$ = normal to slip plane

$\bar b$ = slip direction



$\underset{\sim}{\sigma} = \sigma_{ij}$: GENERAL STRESS STATE IN CRYSTAL AXES.

$\tau_r = \sigma'_{12} = n_i b_j \sigma_{ij}$: RESOLVED SHEAR ON PLANE $\bar n$ IN THE DIRECTION OF $\bar b$.

SCHMID LAW : SLIP IS ACTIVATED WHEN

$$\tau_r = \tau_{critical} \quad , \text{ OTHERWISE } \tau_r < \tau_c$$

KINEMATICS : THE RESULTANT PLASTIC SHEAR IN THE SYSTEM IS $d\gamma^{(s)} = d\varepsilon'_{12}$

AND WHEN EXPRESSED IN CRYSTAL AXES GIVES A PLASTIC STRAIN INCREMENT :

$$d\varepsilon_{ij} = \frac{(n_i b_j + n_j b_i)}{2} d\gamma^{(s)}$$

$$= m_{ij} \, d\gamma^{(s)} .$$

ASSUMPTION: PLASTIC DEFORMATION IS ACT-
IVATED BY SHEAR AND DOES NOT DEPEND ON HYDROSTATIC PRESSURE.

$\Rightarrow$ ONLY $\sigma'_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{kk}\delta_{ij}$ MATTERS,
WHERE $\sigma'_{11} + \sigma'_{22} + \sigma'_{33} = 0$.

$\rightarrow$ ONLY 5 INDEPENDENT STRESS COMPONENTS -
WRITE $\underset{\sim}{\sigma}$ AS A VECTOR $\bar{\sigma} = (\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5)$

SHEAR STRAIN HAS NO VOLUME CHANGES ASSOC-
IATED

$$\Rightarrow \quad \frac{\Delta V}{V} = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} = 0.$$

$\Rightarrow$ ONLY 5 INDEPENDENT STRAIN COMPONENTS -
WRITE $\underset{\sim}{\varepsilon}$ AS A VECTOR $\bar{\varepsilon} = (\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_5)$.

ANY COMBINATION OF STRESS AND STRAIN COMPONENT CAN BE CHOSEN, PROVIDED THAT THE PLASTIC ENERGY REMAINS INVARIANT.

$$dW = \sigma_{ij}\, d\varepsilon_{ij} = \sigma_k\, d\varepsilon_k.$$

WHERE $i, j = 1,3$
AND $k = 1,5$.

② ... GIVES THE SAME FORM
FOR STRESS AND STRAIN VECTORS IS

$$\bar{\sigma} = \left(\frac{\sqrt{3}}{\sqrt{2}}\sigma'_{33},\ \frac{\sigma_{22}-\sigma_{11}}{\sqrt{2}},\ \sqrt{2}\,\sigma_{32},\ \sqrt{2}\,\sigma_{13},\ \sqrt{2}\,\sigma_{12}\right).$$

$$\sigma'_{33} = \left(\frac{\sigma_{33}-\sigma_{11}}{2} + \frac{\sigma_{33}-\sigma_{22}}{2}\right)\cdot\frac{1}{3}$$

$$\bar{\varepsilon} = \left(\frac{\sqrt{3}}{\sqrt{2}}\varepsilon_{33},\ \frac{\varepsilon_{22}-\varepsilon_{11}}{\sqrt{2}},\ \sqrt{2}\,\varepsilon_{23},\ \sqrt{2}\,\varepsilon_{13},\ \sqrt{2}\,\varepsilon_{12}\right)$$

- THE RESOLVED SHEAR STRESS ADOPTS THE FORM.

$$\tau_c^{(s)} = n_i^{(s)} b_j^{(s)} \sigma_{ij} = m_k^{(s)} \sigma_k \qquad (*) \quad (k=1,5)$$

- THE KINEMATIC RELATION BECOMES

$$d\varepsilon_k = m_{jk}^{(s)}\, d\gamma^{(s)} = m_k^{(s)}\, d\gamma^{(s)} \qquad (**) \quad (k=1,5)$$

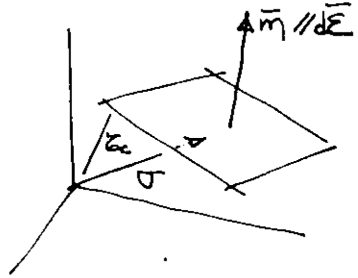
WHERE $\bar{m} = \left(\sqrt{\frac{3}{2}}\, n_3 b_3,\ \frac{n_2 b_2 - n_1 b_1}{\sqrt{2}},\ \frac{n_2 b_3 + n_3 b_2}{\sqrt{2}},\ \dots, \dots\right)$

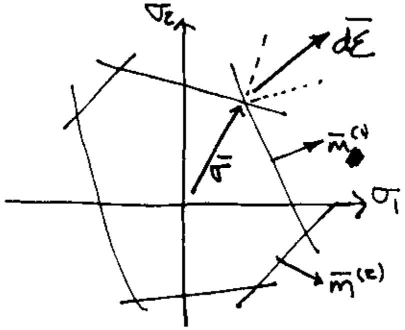
IT IS EVIDENT FROM (**) THAT IF WE IMPOSE FIVE ARBITRARY STRAIN COMPONENTS $d\varepsilon_k$ WE NEED FIVE INDEPENDENT SLIP SYSTEMS TO BE ACTIVE SIMULTANEOUSLY, SUCH THAT:

$$d\varepsilon_k = m_k^{(s)}\, d\gamma^{(s)} \qquad (k=1,5) \quad (s=1,5)$$

(5×5 linear system in unknowns $d\gamma^{(s)}$).

THE CONDITION OF ACTIVATION (EQ. (*)) IS THE EQUATION OF A PLANE IN 5-DIMENSIONAL STRESS-STRAIN SPACE, AT A DISTANCE τ_c FROM THE ORIGIN.
EQ. (**) IMPLIES THAT THE RESULTANT STRAIN VECTOR IS PERPENDICULAR TO THAT PLANE.





- EACH SLIP SYSTEM DEFINES A PLANE
- THE CONDITION $\tau_r^{(s)} \leq \tau_c^{(s)}$ REQUIRES THAT THE STRESS ~~.........~~ HAS TO REMAIN BOUNDED BY THE INNER ENVELOPE DEFINED BY THOSE PLANES
- THE INNER ENVELOPE IS THE SCYS.
- THE CONDITION OF 5 SYSTEMS BEING SIMULTANEOUSLY ACTIVE REQUIRES BEING AT THE INTERSECTION OF 5 PLANES : A VERTEX.
- THE ACTIVE VERTEX CONTAINS $d\bar{E}$ WITHIN ITS CONE OF NORMAL OR, EQUIVALENTLY, IS THE ONE THAT MAXIMICES THE PLASTIC WORK : $\bar{\sigma}^{V} \cdot d\bar{E} = \text{maximum}!$

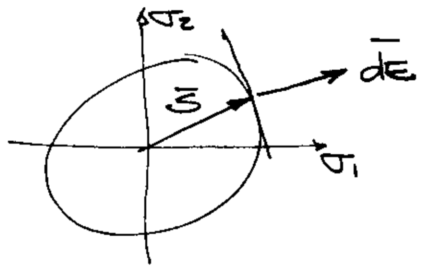
SINCE STRESS AND STRAIN IN THE POLYCRYST... ARE GIVEN AS AN AVERAGE OVER ALL GRAINS

$$S_k = \sum_{\text{grains}} \sigma_k^{gr} \, w^{gr}$$

$$dE_k = \sum_{\text{grains}} d\varepsilon_k^{gr} \, w^{gr}$$

THE PCYS, DEFINED AS THE LOCUS OF POINTS ... STRESS SPACE WHICH LEAD TO PLASTIC FLOW ... THE POLYCRYSTAL, HAS SIMILAR PPTIES.

THE NORMALITY RULE STATES THAT THE RESUL... ANT STRAIN $d\bar{E}$ IS NORMAL TO THE PCY... AT THAT POINT, SO PROVIDING A UNIVOCA... RELATION BETWEEN STRESS AND STRAIN



DISADVANTAGE OF THE BISHOP-HILL APPROACH:

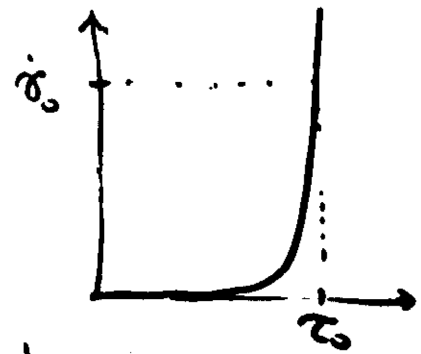
THE VERTICES OF THE SCYS HAVE TO BE KNO... IN ADVANCE.
THEY HAVE TO BE RECALCULATED WHEN THE CRITICAL STRESSES VARY AND ALSO IF DIFFEREN... SLIP OR TWINNING SYSTEMS ARE CONSIDERED T... BE ACTIVE.

(FOLLOW 3 TRANSPARENCIES)

A RATE SENSITIVE VISCO-PLASTIC SINGLE CRYSTAL CONSTITUTIVE EQ.

$$\frac{\dot{\gamma}^s}{\dot{\gamma}_0} = \left[\frac{\tau^s}{\tau_0^s}\right]^{1/m} = \left[\frac{m_{ij} S_{ij}}{\tau_0^s}\right]^{1/m}$$

where $m \ll 1$: rate sensitivity



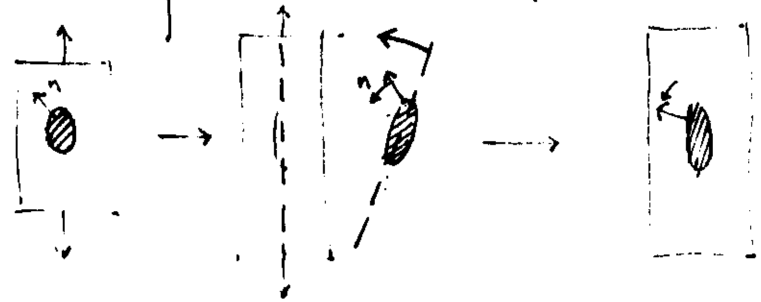
CONSTITUTIVE LAW

$$\boxed{\dot{\varepsilon}_{ij} = \sum_s m_{ij}^s \dot{\gamma}^s = \sum_s m_{ij}^s \left[\frac{m_{kl}^s S_{kl}}{\tau_0^s}\right]^{1/m}}$$

Given $\dot{\varepsilon}_{ij}$ solve for S_{kl} and use it to calculate $\dot{\gamma}^s$ <u>without ambiguity</u>.

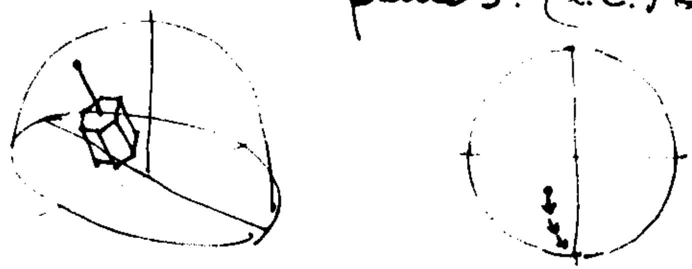
REORIENTATION BY SLIP - TEXTURE

The case of the tensile test:



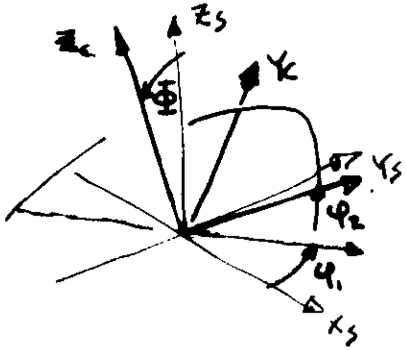
CRYSTAL REORIENTATION

<u>POLE FIGURE</u> : orientations of a family of planes. (i.e.) basal poles).



<u>ORIENTATION DISTRIBUTION FUNCTION.</u>

Density of grains whose crystal axes are within a certain interval in orientation space.



$\varphi_1, \phi, \varphi_2$: Euler angles

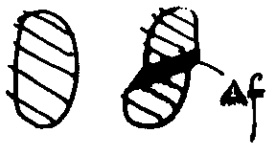
$g(\varphi_1, \phi, \varphi_2) \to$ O.D.F.

REORIENTATION BY TWINNING

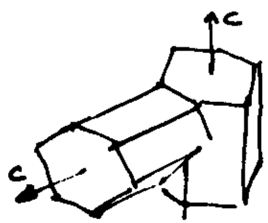
CHARACTERISTICS OF TWINNING

1) Discrete "non-continuous" reorientation.
2.) Unidirectional. !!
3) Microscopic mechanisms uncertain.
4) Stress activated but not necessarily by a critical shear ¿ normal stress ?
5) Associated volume fraction.

$$\Delta f = \frac{\Delta \gamma^{tw}}{S}$$

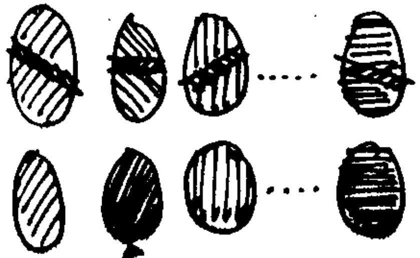


6) Stress relaxation effects → residual stress evidence.
7) Common in hexagonals and lower symmetry crystals.



MODELIZATION OF TWINNING (CLASSICAL).

PROBLEM: Keep track of the twinned volume fra[ction]



whole grain is reoriented (random

UP TO NOW WE KNOW HOW TO DEAL WITH THE DEFORMATION, STRESS AND REORIENTATION OF THE SINGLE CRYSTAL PROVIDED THAT WE KNOW THE STRAIN INCREMENT (AS A TENSOR) BY WHICH THE CRYSTAL DEFORMS.

THE VALUE OF THAT INCREMENT $d\bar{\varepsilon}^{g}$ DEPENDS ON THE MODEL OF POLYCRYSTAL DEFORMATION BEING USED.

* TAYLOR - BISHOP - HILL : IMPOSE SAME STRA[IN] TO EVERY GRAIN : $d\varepsilon^{g}_{k} = d\varepsilon_{k}$

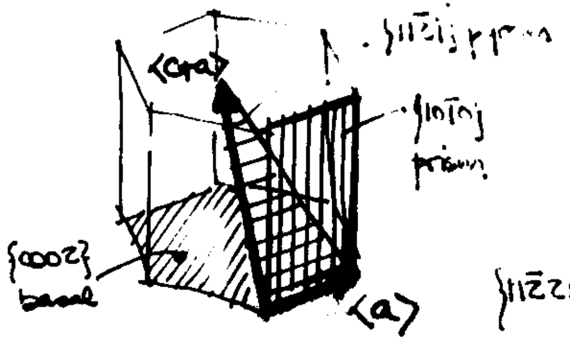
* RELAXED CONSTRAINTS : IMPOSE SOME OF TH[E] STRAIN COMPONENTS EQUAL IN EVERY GRAIN - THE COMPLEMENTARY STRESS COMPONENTS ARE IMPOSED EQUAL TO ZERO

* SELF CONSISTENT : ALLOW FOR DIFFERENT STRESS AND STRAIN IN EACH GRAIN AND FULFILL BOUNDARY CONDITIONS IN AVERAGE.

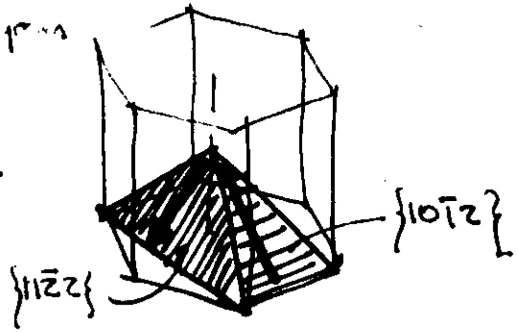
PLASTIC DEFORMATION OF HEXAGONAL CLOSE PACKED MATERIALS.

Deformation modes in Zirconium alloys

Slip modes



Twinning modes



→ $\langle a \rangle$ prismatic
$\langle a \rangle$ pyramidal
$\langle c+a \rangle$ pyramidal

$\langle a \rangle$ basal (not observed)

→ $\{10\bar{1}2\}$ tensile twins
$\{11\bar{2}2\}$ compressive twins

VOLUME FRACTION TRANSFER

- Cells in Euler space - Uniform density in each one.
- "Rigid" displacement of the cell because of reorientation.
- Transference of vol. fractions to neighboring cells with conservation of total mass.

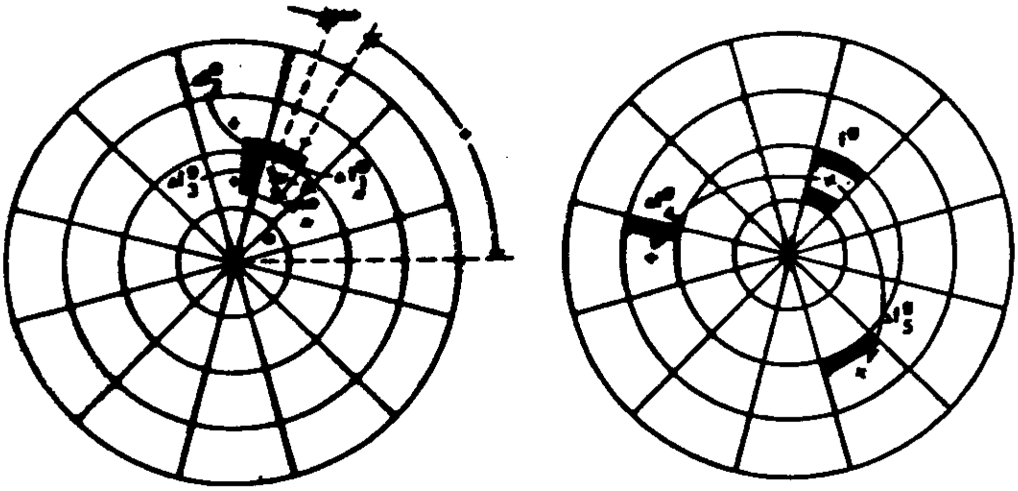
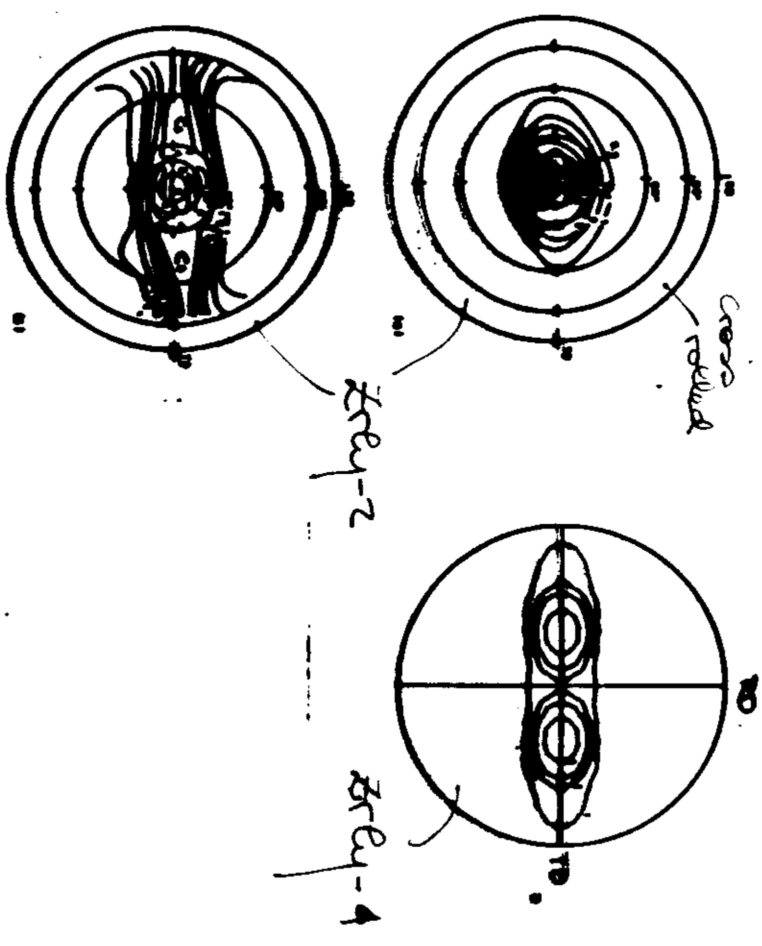


Figure 1 : Schematic representation of volume fraction transfer due to (a) slip reorientation and (b) twinning reorientation for the two dimensional Euler subspace describing the orientation of the basal poles.

→ Fixed orientations but varying volume fractions
→ Accounts exactly for the twinned fraction.

7

Experimental Zircaloy textures
Rolling - Basal poles (c or z)



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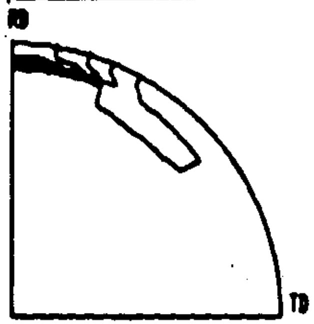
CALCULATED TEXTURE AFTER 50% ROLLING (I

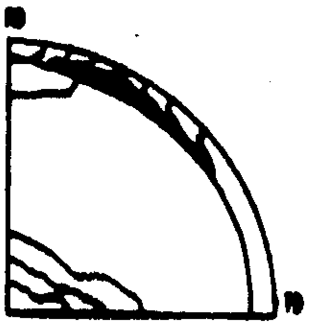
EFFECT OF INCLUDING TWINNING

TRANSFER

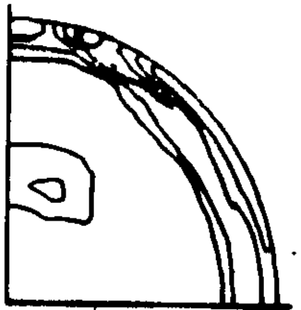


RC - CRSS 01 - PR PYc+a

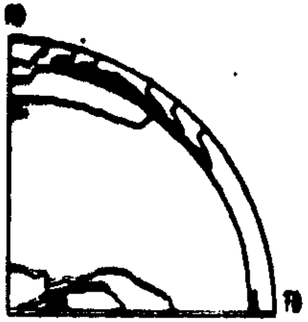
LAPP



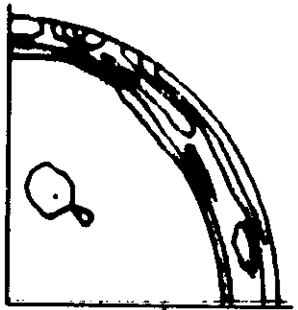
RC - CRSS 01 - PR - PYc+a - TT1



PR / PYc(c+a) / TT1



RC - CRSS 01 - PR (PYa) TT1 CT1

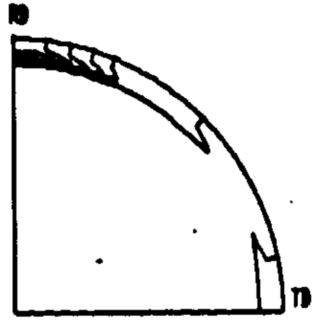


PR/ PY(c+a)/TT1 /CT1

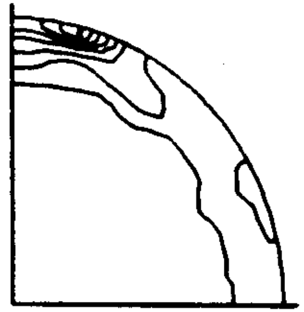
EFFECT OF PYRAMIDAL <a>.

TRANSFER

LAPP

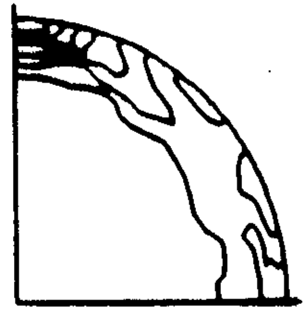


PC - CRSS 01 - PR - PYa - PYc+a

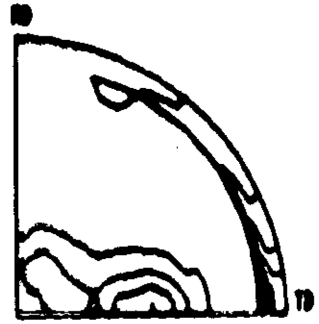


PR PY(a) PYc(c+a)

PC-CRSS 01-PR PYa PYc+a TT1 CT1



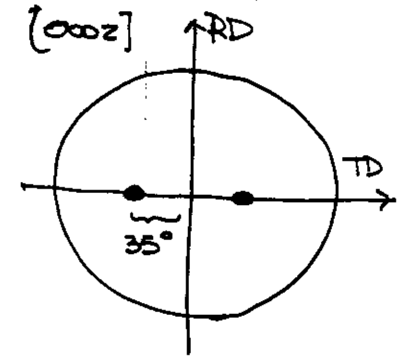
PR/PY(a)/PY(c+a)/TT1/CT1



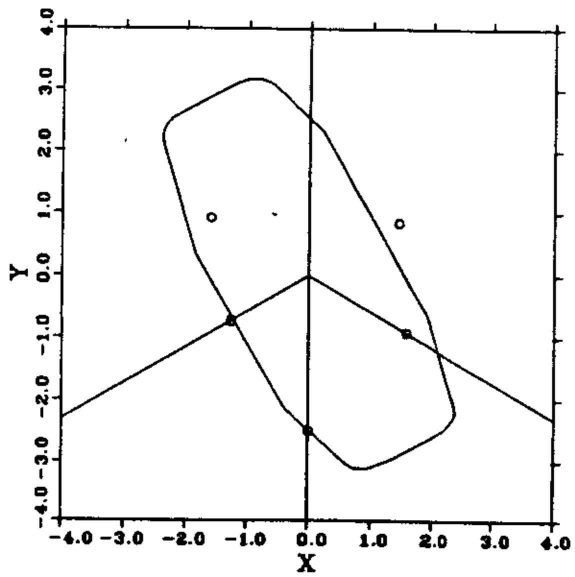
RC - CRSS 01 - PR PYa TT1 CT1

PR / PY(a)/TT1/CT1

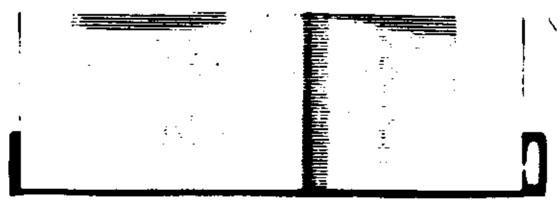
11/09/87 (a3)
2 grains



$\tau^{PR} = 0.50$
$\tau^{T.TW.} = 0.75$
$\tau^{C.TW} = 0.85$
$\tau^{PYR} = 1.00$.



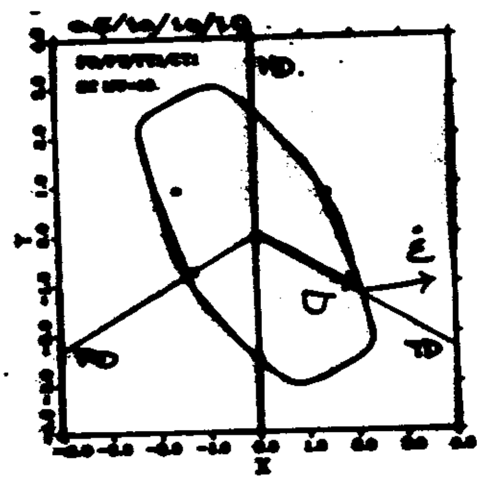
75%

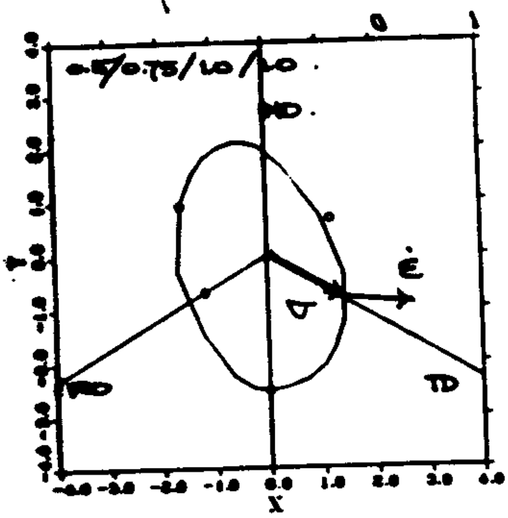


YIELD LOCI OF ROLLED ZIRCALOY-4

<a> prismat.
<a+c> pyramidal
tensile twins
compressive twins

<a> prismatic
<a> pyramidal
tensile twins
compressive twins.





negative Lankford coefficient !!

$R = \frac{\varepsilon_T}{\varepsilon_L}$

CONCLUSIONS

* Hexagonal materials present a challenge as far as the prediction of texture development is concerned.

* The active deformation modes and their interactions (hardening) are not known in detail. Reliable deformation codes may provide information about them (i.e. our results indicate that some amount of pyramidal <a> may be present).

* Twinning is an ubiquitous mechanism and has yet to be understood and modeled properly.

* Self-consistent models seem to be better suited for treating hexagonals. Nevertheless, they are not of much use unless the [illegible] conditions are fulfilled.

* The "volume fraction transfer scheme" seems to be a more reasonable alternative for accounting for twinning reorientation.