# SSND112 – Rotation of network and great deformations on a monocrystal

**Summary:**

One carries out, on a problem reduced to the material point, a traction on a monocrystal

Modeling a: this modeling makes it possible to validate the behavior `MONOCRYSTAL of the type` $CFC$ . in great deformations

Modeling b: this modeling makes it possible to validate the behavior `MONOCRYSTAL of the type` $CFC$ . in small deformations with taking into account of the rotation of the crystal lattice

Modeling C: this modeling uses the behavior `MONOCRYSTAL of the type` $CFC$ . in small deformations for qualitative comparison with modelings A and B.

Modeling D: this modeling uses the behavior `MONOCRYSTAL of the type` $CC$ . in great deformations.

Modeling E: this modeling makes it possible to validate the behavior `MONOCRYSTAL of the type` $CFC$ . in great deformations, in the same way that modeling A, but with the behavior $\mathrm{CFC\_IRRA}$

# 1 Problem of reference

## 1.1 Geometry

It is about a material point, representative of a stress and strain state homogeneous. It can be simulated by an element of volume represented by only one finite element.

## 1.2 Properties of materials

### 1.2.1 Coefficients relating to isotropic elasticity

$$E=173000MPa\,,\ \nu=0.3\quad \mu=\frac{E}{2(1+\nu)}$$

### 1.2.2 Coefficients of the crystalline law MONO_DD_CFC (modelings A, B, C, E)

$A=0.13$
$B=0.005$
$Y=2.5\mathrm{E}-7\,mm\,(2.5\,Angstr\ddot{o}m)$
$\tau_f=20.$
$n=50.$
$\dot{\gamma}_0=10^{-3}$
$\rho_{ref}=10^6\,mm^{-2}$

$\alpha=0.35$
$\beta=2.5410^{-7}(2.54\,Angstr\ddot{o}m)$

The matrix of interaction is that definite for MONO_DD_CFC [R5.03.11].
The family of systems of slip is octahedral ( $CFC$ )

The coefficients related to the irradiation (modeling E) are:

$\alpha^{loops}=0\quad \phi^{loops}=0.001\quad \alpha^{voids}=0\quad \rho^{voids}=1.e3$
$\rho_{sat}=4\,\rho_0 b^2\quad \phi_{sat}=0.04\quad \xi_{irra}=10^7\quad \zeta_{irra}=10^7$ with $\rho_0=10^6\,mm^{-2}$

The internal variables representing the density of dislocations are initialized with $\rho_0 * b^2$
Those which are related to the irradiation have as initial values: $\rho_s^{loops}=2\,\rho_0 b^2\quad \phi_s^{voids}=0.001$

### 1.2.3 Coefficients of the crystalline law MONO_DD_CC (modeling D)

$D_{LAT}=1.0$ ,
$K_{BOLTZ}=8.62\mathrm{E}-05,$
$GAMMA0=1.\mathrm{E}-3, TAU_F=2.\mathrm{E}7,\ TAU_0=3.63,$
$RHO_{MOB}=1.\mathrm{E}11,$
$K_F=30.0, K_{SELF}=100.0,$
$B=2.48\mathrm{E}-10, DELTAG0=0.84, D=1.\mathrm{E}-08,$
$N=20.0, BETA=0.2,$
$GH=1.\mathrm{E}11, Y_{AT}=1.00\mathrm{E}-09,$

The matrix of interaction is constuite starting from the following values
$H1=0.1024$, $H2=0.7$, $H3=0.1$, $H4=0.1$, $H5=0.1$ $H6=0.1$,

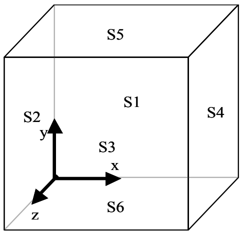
The family of systems of slip is cubique1 ( $CC$ ).

The internal variables representing the density of dislocations are initialized with $\rho_0=10^5 mm^{-2}$

The formulation used here is formulation 1 (selected using parameter DELTA1=0) (cf [R5.03.11]

## 1.3 Boundary conditions and loadings

The cubic element of volume on side $1\mathrm{m}$ is subjected to a homogeneous simple tensile test, in deformations imposées.1 HEXA8.




The imposed loading is the following:

- The face $S1$ is blocked according to the direction $z$
- The face $S3$ a displacement undergoes of $0{,}2\,mm$ in $0.2\,s$ and in 100 increments.
- displacements according to $X$ and $Y$ point origin are worthless
- a stiffness being worth $10^4 N/m$ according to $Y$ is added to the point origin, via a discrete element, pour to allow a quasi-free rotation around $Z$

## 1.4 Initial conditions

Worthless constraints and deformations. Initial density of dislocations: $\rho_0=10^6 mm^{-2}$

# 2 Reference solution

It rests on [bib.1] and [v6.08.110]. In the field as of small deformations, the tensor of the constraints $\boldsymbol{\sigma}$ being uniaxial, one can calculate for each system of slip, the scission solved by: $\tau_s=\boldsymbol{\sigma}:\boldsymbol{\mu}_s$ with $\boldsymbol{\mu}_s$ the tensor of orientation defined by: $(m_s)_{ij}=\frac{1}{2}((n_s)_i\cdot(l_s)_j+(l_s)_i\cdot(n_s)_j)$ , $\mathbf{n_s}$ indicating the normal with the slip surface of the system $s$ and $\mathbf{l_s}$ direction of slip. The evolution of the plastic slip is given for each system $s$ by (cf [R5.03.11]):

Case of $CFC$ : For the orientation chosen, that is to say 1-5-9, the initial factors of Schmid, connecting the tensor of the constraints to the various solved scissions $\tau_s$ are, for the 12 octahedral systems:

$$[0.45784855, 0.22892428, 0.22892428, 0.15261618, 0.26707832, 0.11446214, \\ 0.19840104, 0.29760156, 0.4960026, 0.04578486, 0.11446214, 0.16024699]$$

It is thus noted that the first system of activated slip will be number 9 ( $A3$ ), and the second will be number 1 (either $B4$ ).

In great deformations, or taking of account the rotation of network, one must see appearing for a noninfinitesimal deformation a third system of slip, $C1$ (12th system in Code_Aster) whose activity grows in an important way, while viscoplastic slip of the system $A3$ do not evolve any more [2].

## 2.1 Bibliographical references

[1] N.Rupin Notes EDF-R&D: HT24 - 2010 - 01128 "implementation of have new constitutive law based one dislocation dynamics for FCC materials".

[2] Simulation of the mechanical answer of an austenitic stainless steel using crystalline calculations NR. Toff, J.M. Proix, F. Latourte, G. Monnet, communication with the 10th National Conference in Calculation of the Structures, May 9th-13th, 2011, Peninsula of Giens (VAr).

# 3 Modeling A

## 3.1 Characteristics of modeling

The behavior is MONOCRYSTAL, in great deformations (DEFORMATION=' SIMO_MIEHE')

## 3.2 Sizes tested and results

### 3.2.1 Values tested

Small deformations, comparison with modeling C.

| Variable | Moments $(s)$ | Reference | Tolerance |
|---|---|---|---|
| $E_{zz}$ EPSG_ELGA | 0.02 | 0.02023 | 0.001 |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 0.02 | 114,125 | 0.01 |
| $\rho_1$ VARI_ELGA/V7) | 0.02 | 9.8085E-07 | 0.005 |
| $\gamma_1$ VARI_ELGA/V8) | 0.02 | 0.0385 | 0.005 |
| $\rho_9$ VARI_ELGA/V31) | 0.02 | 1.0741E-07 | 0.13 |
| $\gamma_9$ VARI_ELGA/V32) | 0.02 | 1.04944E-03 | 0.33 |
| test of nonregression on the two last values | | | |
| $\rho_9$ VARI_ELGA/V31) | 0.02 | 9.30093E-08 | 0.001 |
| $\gamma_9$ VARI_ELGA/V32) | 0.02 | 7.0377E-04 | 0.001 |

Great deformations, comparison with modeling B

| Variable | Moments $(s)$ | Reference | Tolerance |
|---|---|---|---|
| $E_{zz}$ EPSG_ELGA | 0.2 | 0.22385 | 0.002 |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 0.2 | 320,153 | 0.09 |
| $\rho_1$ VARI_ELGA/V7) | 0.2 | 1.731E-05 | 0.18 |
| $\gamma_1$ VARI_ELGA/V8) | 0.2 | 0.31346 | 0.06 |
| $\rho_9$ VARI_ELGA/V31) | 0.2 | 8.37E-07 | 0.06 |
| $\gamma_9$ VARI_ELGA/V32) | 0.2 | 0.010410 | 0.06 |
| $\rho_{12}$ VARI_ELGA/V40) | 0.2 | 1.719E-05 | 0.24 |
| $\gamma_{12}$ VARI_ELGA/V41) | 0.2 | 0.11118 | 0.21 |
| test of nonregression | | | |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 0.2 | 293,247 | 0.001 |
| $\rho_1$ VARI_ELGA/V7) | 0.2 | 1.425E-05 | 0.001 |
| $\gamma_1$ VARI_ELGA/V8) | 0.2 | 0.297258 | 0.001 |
| $\rho_9$ VARI_ELGA/V31) | 0.2 | 7.87472E-07 | 0.001 |
| $\gamma_9$ VARI_ELGA/V32) | 0.2 | 9.79517E-03 | 0.001 |
| $\rho_{12}$ VARI_ELGA/V40) | 0.2 | 1.309E-05 | 0.001 |
| $\gamma_{12}$ VARI_ELGA/V41) | 0.2 | 0.088585 | 0.001 |

# 4 Modeling B

## 4.1 Characteristics of modeling

The behavior is MONOCRYSTAL, in small deformations (DEFORMATION=' PETIT'), but with rotation of crystal lattice (ROTA_RESEAU=' CALC' in DEFI_COMPOR).

## 4.2 Sizes tested and results

### 4.2.1 Values tested

Small deformations, comparison with modeling C.

| Variable | Moments $(s)$ | Reference | Tolerance |
|---|---|---|---|
| $E_{zz}$ EPSG_ELGA | 0.02 | 0.02023 | 0.001 |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 0.02 | 114,125 | 0.011 |
| $\rho_1$ VARI_ELGA/V7) | 0.02 | 9.8085E-07 | 0.01 |
| $\gamma_1$ VARI_ELGA/V8) | 0.02 | 0.0385 | 0.012 |
| $\rho_9$ VARI_ELGA/V31) | 0.02 | 1.0741E-07 | 0.13 |
| $\gamma_9$ VARI_ELGA/V32) | 0.02 | 1.04944E-03 | 0.30 |
| test of nonregression on the two last values | | | |
| $\rho_9$ VARI_ELGA/V31) | 0.02 | 9.5373E-08 | 0.001 |
| $\gamma_9$ VARI_ELGA/V32) | 0.02 | 7.6027E-04 | 0.001 |

Great deformations, not regression

| Variable | Moments $(s)$ | Reference | Tolerance |
|---|---|---|---|
| $E_{zz}$ EPSG_ELGA | 0.2 | 0.22385 | 0.001 |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 0.2 | 320,153 | 0.001 |
| $\rho_1$ VARI_ELGA/V7) | 0.2 | 1.731E-05 | 0.001 |
| $\gamma_1$ VARI_ELGA/V8) | 0.2 | 0.31346 | 0.001 |
| $\rho_9$ VARI_ELGA/V31) | 0.2 | 8.37E-07 | 0.001 |
| $\gamma_9$ VARI_ELGA/V32) | 0.2 | 0.010410 | 0.001 |
| $\rho_{12}$ VARI_ELGA/V40) | 0.2 | 1.719E-05 | 0.001 |
| $\gamma_{12}$ VARI_ELGA/V41) | 0.2 | 0.11118 | 0.001 |

# 5 Modeling C

## 5.1 Characteristics of modeling

The behavior is MONOCRYSTAL, in small deformations (DEFORMATION=' PETIT')

## 5.2 Sizes tested and results

### 5.2.1 Values tested

Imposed deformation of 0.02, test of nonregression.

| Variable | Moments $(s)$ | Reference | Tolerance |
|---|---|---|---|
| $E_{zz}$ EPSG_ELGA | 0.02 | 0.02023 | 0.001 |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 0.02 | 114,125 | 0.001 |
| $\rho_1$ VARI_ELGA/V7) | 0.02 | 9.8085E-07 | 0.001 |
| $\gamma_1$ VARI_ELGA/V8) | 0.02 | 0.0385 | 0.001 |
| $\rho_9$ VARI_ELGA/V31) | 0.02 | 1.0741E-07 | 0.001 |
| $\gamma_9$ VARI_ELGA/V32) | 0.02 | 1.04944E-03 | 0.001 |

Imposed deformation of 0.2, test of nonregression.

| Variable | Moments $(s)$ | Reference | Tolerance |
|---|---|---|---|
| $E_{zz}$ EPSG_ELGA | 0.2 | 0.22444 | 0.001 |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 0.2 | 230.7133 | 0.001 |
| $\rho_1$ VARI_ELGA/V7) | 0.2 | 1.49E-05 | 0.001 |
| $\gamma_1$ VARI_ELGA/V8) | 0.2 | 0.3567 | 0.001 |
| $\rho_9$ VARI_ELGA/V31) | 0.2 | 6.30676E-06 | 0.001 |
| $\gamma_9$ VARI_ELGA/V32) | 0.2 | 0.05493 | 0.001 |
| $\rho_{12}$ VARI_ELGA/V40) | 0.2 | 6.45160E-08 $=\rho_0$ | 0.001 |
| $\gamma_{12}$ VARI_ELGA/V41) | 0.2 | 0 | 0.001 |

This modeling also comprises two additional calculations:

– the first with a matrix of interaction provided in a table:

| syst | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0,124 | 0,124 | 0,124 | 0,625 | 0,137 | 0,137 | 0,137 | 0,122 | 0,070 | 0,137 | 0,070 | 0,122 |
| 2 | 0,124 | 0,124 | 0,124 | 0,137 | 0,070 | 0,122 | 0,625 | 0,137 | 0,137 | 0,137 | 0,122 | 0,070 |
| 3 | 0,124 | 0,124 | 0,124 | 0,137 | 0,122 | 0,070 | 0,137 | 0,070 | 0,122 | 0,625 | 0,137 | 0,137 |
| 4 | 0,625 | 0,137 | 0,137 | 0,124 | 0,124 | 0,124 | 0,122 | 0,137 | 0,070 | 0,122 | 0,070 | 0,137 |
| 5 | 0,137 | 0,070 | 0,122 | 0,124 | 0,124 | 0,124 | 0,070 | 0,137 | 0,122 | 0,137 | 0,137 | 0,625 |
| 6 | 0,137 | 0,122 | 0,070 | 0,124 | 0,124 | 0,124 | 0,137 | 0,625 | 0,137 | 0,070 | 0,122 | 0,137 |
| 7 | 0,137 | 0,625 | 0,137 | 0,122 | 0,070 | 0,137 | 0,124 | 0,124 | 0,124 | 0,122 | 0,137 | 0,070 |
| 8 | 0,122 | 0,137 | 0,070 | 0,137 | 0,137 | 0,625 | 0,124 | 0,124 | 0,124 | 0,070 | 0,137 | 0,122 |
| 9 | 0,070 | 0,137 | 0,122 | 0,070 | 0,122 | 0,137 | 0,124 | 0,124 | 0,124 | 0,137 | 0,625 | 0,137 |
| 10 | 0,137 | 0,137 | 0,625 | 0,122 | 0,137 | 0,070 | 0,122 | 0,070 | 0,137 | 0,124 | 0,124 | 0,124 |
| 11 | 0,070 | 0,122 | 0,137 | 0,070 | 0,137 | 0,122 | 0,137 | 0,137 | 0,625 | 0,124 | 0,124 | 0,124 |
| 12 | 0,122 | 0,070 | 0,137 | 0,137 | 0,625 | 0,137 | 0,070 | 0,122 | 0,137 | 0,124 | 0,124 | 0,124 |

- the second uses moreover 12 systems of slip given in a table

| syst | n1 | n2 | n3 | m1 | m2 | m3 |
|---|---|---|---|---|---|---|
| 1 | 1,00 | 1,00 | 1,00 | -1.00 | 0.00 | 1,00 |
| 2 | 1,00 | 1,00 | 1,00 | 0.00 | -1.00 | 1,00 |
| 3 | 1,00 | 1,00 | 1,00 | -1.00 | 1,00 | 0.00 |
| 4 | 1,00 | -1.00 | 1,00 | -1.00 | 0.00 | 1,00 |
| 5 | 1,00 | -1.00 | 1,00 | 0.00 | 1,00 | 1,00 |
| 6 | 1,00 | -1.00 | 1,00 | 1,00 | 1,00 | 0.00 |
| 7 | -1.00 | 1,00 | 1,00 | 0.00 | -1.00 | 1,00 |
| 8 | -1.00 | 1,00 | 1,00 | 1,00 | 1,00 | 0.00 |
| 9 | -1.00 | 1,00 | 1,00 | 1,00 | 0.00 | 1,00 |
| 10 | -1.00 | -1.00 | 1,00 | -1.00 | 1,00 | 0.00 |
| 11 | -1.00 | -1.00 | 1,00 | 1,00 | 0.00 | 1,00 |
| 12 | -1.00 | -1.00 | 1,00 | 0.00 | 1,00 | 1,00 |

– the values provided for the matrix of interaction and the systems of slip are identical to the values of matrix of interaction and the systems of the selected behavior (cf [R5.03.11) It is thus checked that the results are the same ones.

# 6 Modeling D

## 6.1 Characteristics of modeling

The behavior is MONOCRYSTAL, the viscoplastic flow is of type MONO_DD_CC, in great deformations (DEFORMATION=' SIMO_MIEHE')

## 6.2 Sizes tested and results

### 6.2.1 Values tested

Great deformations, not regression.

The system of principal slip is number 5 ( $D1$ ) and the secondary is the 8 ( $A6$ )

| Variable | Moments $(s)$ | Reference |
|---|---|---|
| $E_{zz}$ EPSG_ELGA | 4000 | 0.48758 |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 4000 | 269.278 |
| $\rho_5$ VARI_ELGA/V19) | 4000 | 4.71621E+07 |
| $\gamma_5$ VARI_ELGA/V20) | 4000 | -0.42962 |
| $\rho_8$ VARI_ELGA/V28) | 4000 | 3.84436E+07, |
| $\gamma_8$ VARI_ELGA/V29) | 4000 | 0.261159 |

# 7 Modeling E

## 7.1 Characteristics of modeling

The behavior is MONOCRYSTAL, in great deformations (DEFORMATION=' SIMO_MIEHE'), in a way similar to modeling A, with a crystalline behavior which takes into account the irradiation

## 7.2 Sizes tested and results

### 7.2.1 Values tested

Small deformations, comparison with modeling C.

| Variable | Moments $(s)$ | Reference | Tolerance |
|---|---|---|---|
| $E_{zz}$ EPSG_ELGA | 0.02 | 0.02023 | 0.001 |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 0.02 | 114,125 | 0.01 |
| $\rho_1$ VARI_ELGA/V7) | 0.02 | 9.8085E-07 | 0.005 |
| $\gamma_1$ VARI_ELGA/V8) | 0.02 | 0.0385 | 0.005 |
| $\rho_9$ VARI_ELGA/V31) | 0.02 | 1.0741E-07 | 0.13 |
| $\gamma_9$ VARI_ELGA/V32) | 0.02 | 1.04944E-03 | 0.33 |
| test of nonregression on the two last values | | | |
| $\rho_9$ VARI_ELGA/V31) | 0.02 | 9.30093E-08 | 0.001 |
| $\gamma_9$ VARI_ELGA/V32) | 0.02 | 7.0377E-04 | 0.001 |

Great deformations, comparison with modeling B

| Variable | Moments $(s)$ | Reference | Tolerance |
|---|---|---|---|
| $E_{zz}$ EPSG_ELGA | 0.2 | 0.22385 | 0.002 |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 0.2 | 320,153 | 0.09 |
| $\rho_1$ VARI_ELGA/V7) | 0.2 | 1.731E-05 | 0.18 |
| $\gamma_1$ VARI_ELGA/V8) | 0.2 | 0.31346 | 0.06 |
| $\rho_9$ VARI_ELGA/V31) | 0.2 | 8.37E-07 | 0.06 |
| $\gamma_9$ VARI_ELGA/V32) | 0.2 | 0.010410 | 0.06 |
| $\rho_{12}$ VARI_ELGA/V40) | 0.2 | 1.719E-05 | 0.24 |
| $\gamma_{12}$ VARI_ELGA/V41) | 0.2 | 0.11118 | 0.21 |
| test of nonregression | | | |
| $\sigma_{zz}$ ( $Mpa$ ) SIEF_ELGA | 0.2 | 293,247 | 0.001 |
| $\rho_1$ VARI_ELGA/V7) | 0.2 | 1.425E-05 | 0.001 |
| $\gamma_1$ VARI_ELGA/V8) | 0.2 | 0.297258 | 0.001 |
| $\rho_9$ VARI_ELGA/V31) | 0.2 | 7.87472E-07 | 0.001 |
| $\gamma_9$ VARI_ELGA/V32) | 0.2 | 9.79517E-03 | 0.001 |
| $\rho_{12}$ VARI_ELGA/V40) | 0.2 | 1.309E-05 | 0.001 |
| $\gamma_{12}$ VARI_ELGA/V41) | 0.2 | 0.088585 | 0.001 |

The results are identical to those of modeling A, which is the expected result: the coefficients making it possible to take into account the effect of the irradiation in work hardening are selected worthless here.

# 8 Summary of the results

The results are satisfactory and validate the great deformations of the behavior MONOCRYSTAL.