SSND112 – Rotation of network and large deformations on a Summarized

monocrystal:

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

Modelization a: this modelization allows to validate behavior MONOCRISTAL of the type CFC .en large deformations

Modelization b: this modelization allows to C validate behavior MONOCRISTAL of the type CFC .en small strains with taking into account of the rotation of the crystal lattice

Modelization: this modelization uses behavior MONOCRISTAL of the type CFC .en small strains for qualitative comparison with the modelizations A and B.

Modelization D: this modelization uses behavior MONOCRISTAL of the type CC .en large deformations.

Modelization E: this modelization makes it possible to validate behavior MONOCRISTAL of the type CFC .en large deformations, in the same way that the modelization A, but with the behavior CFC_IRRA

1 Problem of reference

1.1 Geometry

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

1.2 Properties of the materials

1.2.1 Coefficients relating to isotropic elasticity

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

1.2.2 Coefficients of crystalline model MONO_DD_CFC (modelizations A, B, C, E)

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

$\alpha=0.35$
$\beta=2.5410^{-7}(2.54\,Angström)$

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

the coefficients related to the irradiation (modelization E) are:
$\alpha^{loops}=0$ $\phi^{loops}=0.001$ $\alpha^{voids}=0$ $\rho^{voids}=1.e3$
$\rho_{sat}=4\,\rho_0 b^2$ $\phi_{sat}=0.04$ $\xi_{irra}=10^7$ $\zeta_{irra}=10^7$ with $\rho_0=10^6\,mm^{-2}$

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

1.2.3 Coefficients of crystalline model MONO_DD_CC (modelization 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
$H1=0.1024$, $H2=0.7$, $H3=0.1$, $H4=0.1$, $H5=0.1$ $H6=0.1$,

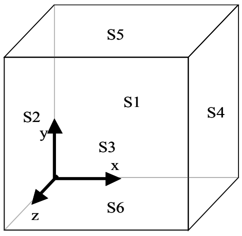
the family of sliding systems is cubique1 (CC).

The local 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 volume element of on the east side 1m subjected to a homogeneous simple traction test, in strains imposées.1 HEXA8.



The imposed loading is the following:

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

1.4 Forced

Initial conditions and null strains. Initial density of dislocations: $\rho_0=10^6 mm^{-2}$

2 Reference solution

It leans on [bib.1] and [v6.08.110]. In the field of the small strains, the tensor of the stresses $\boldsymbol{\sigma}$ being uniaxial, one can calculate for each system of sliding, the scission solved by: $\tau_s=\boldsymbol{\sigma}:\boldsymbol{\mu}_\mathbf{s}$ with $\boldsymbol{\mu}_\mathbf{s}$ the tensor of directional sense 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 norm with the slip surface of the system s and $\mathbf{l_s}$ the direction of sliding. The evolution of the plastic sliding is given for each system s by (cf [R5.03.11]):

Case of CFC : For the directional sense chosen, that is to say 1-5-9, the initial factors of Schmid, connecting the tensor of the stresses to the various solved scissions τ_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 sliding will be number 9 ($A3$), and the second will be number 1 (either $B4$).

In large deformations, or taking into account the rotation of network, one must see appearing for a noninfinitesimal strain a third system of sliding, $C1$ (12th system in Code_Aster) whose activity grows in an important way, while the viscoplastic sliding of the system $A3$ does 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 response of an austenitic stainless steel using crystalline computations N. Toff, J.M. Proix, F. Latourte, G. Monnet, communication with the 10th National Conference in Computation of Structures, May 9th-13th, 2011, Peninsula of Giens (VAr).

3 Modelization A

3.1 Characteristic of the modelization

the behavior is MONOCRISTAL, in large deformations (DEFORMATION=' SIMO_MIEHE')

3.2 Quantities tested and Values

3.2.1 results tested

Small strains, comparison with the Variable modelization C

.	Times (s)	Reference	Tolerance
E_{zz} EPSG_ELGA	0,02	0.02023	0,001
σ_{zz} (Mpa) SIEF_ELGA	0,02	114.125	0,01
ρ_1 VARI_ELGA/V7)	0,02	9.8085E-07	0,005
γ_1 VARI_ELGA/V8)	0,02	0.0385	0,005
ρ_9 VARI_ELGA/V31)	0,02	1.0741E-07	0,13
γ_9 VARI_ELGA/V32)	0,02	1.04944E-03	0,33
test of non regression on two last values			
ρ_9 VARI_ELGA/V31)	0,02	9.30093E-08	0,001
γ_9 VARI_ELGA/V32)	0,02	7.0377E-04	0,001

Large deformations, comparison with the modelization B

Variable	Times (s)	Reference	Tolerance
E_{zz} EPSG_ELGA	0,2	0.22385	0,002
σ_{zz} (Mpa) SIEF_ELGA	0,2	320.153	0,09
ρ_1 VARI_ELGA/V7)	0,2	1.731E-05	0,18
γ_1 VARI_ELGA/V8)	0,2	0.31346	0,06
ρ_9 VARI_ELGA/V31)	0,2	8.37E-07	0,06
γ_9 VARI_ELGA/V32)	0,2	0.010410	0,06
ρ_{12} VARI_ELGA/V40)	0,2	1.719E-05	0,24
γ_{12} VARI_ELGA/V41)	0,2	0.11118	0,21
test of non regression			
σ_{zz} (Mpa) SIEF_ELGA	0,2	293.247	0,001
ρ_1 VARI_ELGA/V7)	0,2	1.425E-05	0,001
γ_1 VARI_ELGA/V8)	0,2	0.297258	0,001
ρ_9 VARI_ELGA/V31)	0,2	7.87472E-07	0,001
γ_9 VARI_ELGA/V32)	0,2	9.79517E-03	0,001
ρ_{12} VARI_ELGA/V40)	0,2	1.309E-05	0,001
γ_{12} VARI_ELGA/V41)	0,2	0.088585	0,001

4 Modelization B

4.1 Characteristic of the modelization

the behavior are MONOCRISTAL, in small strains (DEFORMATION=' PETIT'), but with rotation of crystal lattice (ROTA_RESEAU=' CALC' in DEFI_COMPOR).

4.2 Quantities tested and Values

4.2.1 results tested

Small strains, comparison with the Variable modelization C

.	Times (s)	Reference	Tolerance
E_{zz} EPSG_ELGA	0,02	0.02023	0,001
σ_{zz} (Mpa) SIEF_ELGA	0,02	114.125	0,011
ρ_1 VARI_ELGA/V7)	0,02	9.8085E-07	0,01
γ_1 VARI_ELGA/V8)	0,02	0.0385	0,012
ρ_9 VARI_ELGA/V31)	0,02	1.0741E-07	0,13
γ_9 VARI_ELGA/V32)	0,02	1.04944E-03	0,30
test of non regression on two last values			
ρ_9 VARI_ELGA/V31)	0,02	9.5373E-08	0,001
γ_9 VARI_ELGA/V32)	0,02	7.6027E-04	0,001

Large deformations, non regression

Variable	Times (s)	Reference	Tolerance
E_{zz} EPSG_ELGA	0,2	0.22385	0,001
σ_{zz} (Mpa) SIEF_ELGA	0,2	320.153	0,001
ρ_1 VARI_ELGA/V7)	0,2	1.731E-05	0,001
γ_1 VARI_ELGA/V8)	0,2	0.31346	0,001
ρ_9 VARI_ELGA/V31)	0,2	8.37E-07	0,001
γ_9 VARI_ELGA /V32)	0,2	0.010410	0,001
ρ_{12} VARI_ELGA/V40)	0,2	1.719E-05	0,001
γ_{12} VARI_ELGA/V41)	0,2	0.11118	0,001

5 Modelization C

5.1 Characteristic of the modelization

the behavior is `MONOCRISTAL`, in small strains (`DEFORMATION=' PETIT'`)

5.2 Quantities tested and Values

5.2.1 results tested

imposed Strain of 0.02, test of non regression.

Variable	Times (s)	Reference	Tolerance
E_{zz} EPSG_ELGA	0,02	0.02023	0,001
σ_{zz} (Mpa) SIEF_ELGA	0,02	114.125	0,001
ρ_1 VARI_ELGA/V7)	0,02	9.8085E-07	0,001
γ_1 VARI_ELGA/V8)	0,02	0.0385	0,001
ρ_9 VARI_ELGA/V31)	0,02	1.0741E-07	0,001
γ_9 VARI_ELGA/V32)	0,02	1.04944E-03	0,001

imposed Strain of 0.2, test of non regression.

Variable	Times (s)	Reference	Tolerance
E_{zz} EPSG_ELGA	0,2	0.22444	0,001
σ_{zz} (Mpa) SIEF_ELGA	0,2	230,7133	0,001
ρ_1 VARI_ELGA/V7)	0,2	1.49E-05	0,001
γ_1 VARI_ELGA/V8)	0,2	0.3567	0,001
ρ_9 VARI_ELGA/V31)	0,2	6.30676E-06	0,001
γ_9 VARI_ELGA/V32)	0,2	0.05493	0,001
ρ_{12} VARI_ELGA/V40)	0,2	6.45160E-08 $=\rho_0$	0,001
γ_{12} VARI_ELGA/V41)	0,2	0	0,001

This modelization also comprises two additional computations:

−the first with a matrix of interaction provided in an array:

−the second and the uses moreover 12 sliding systems given in

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

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

–an array the values provided for the matrix of interaction sliding systems are identical to the values of matrix of interaction and of the systems of the selected behavior (cf [R5.03.11) One thus checks that the results are the same ones.

6 Modelization D

6.1 Characteristic of the modelization

the behavior is MONOCRISTAL, viscoplastic flow is of type MONO_DD_CC, in large deformations (DEFORMATION=' SIMO_MIEHE')

6.2 Quantities tested and Values

6.2.1 results tested

Large deformations, non regression.

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

Variable	Times (s)	Reference
E_{zz} EPSG_ELGA	4000	4,85636E-001
σ_{zz} (Mpa) SIEF_ELGA	4000	3,4184E+002
ρ_5 VARI_ELGA/V19)	4000	1,1964E+008
γ_5 VARI_ELGA/V20)	4000	-4,53E-001
ρ_8 VARI_ELGA/V28)	4000	9,18652E+007
γ_8 VARI_ELGA/V29)	4000	2,3728E-001

7 Modelization E

7.1 Characteristic of the modelization

the behavior is MONOCRISTAL, in large deformations (DEFORMATION=' SIMO_MIEHE'), in a way similar to the modelization A, with a crystalline behavior which takes into account the irradiation

7.2 Quantities tested and Values

7.2.1 results tested

Small strains, comparison with the Variable modelization C

.	Times (s)	Reference	Tolerance
E_{zz} EPSG_ELGA	0,02	0.02023	0,001
σ_{zz} (Mpa) SIEF_ELGA	0,02	114.125	0,01
ρ_1 VARI_ELGA/V7)	0,02	9.8085E-07	0,005
γ_1 VARI_ELGA/V8)	0,02	0.0385	0,005
ρ_9 VARI_ELGA/V31)	0,02	1.0741E-07	0,13
γ_9 VARI_ELGA/V32)	0,02	1.04944E-03	0,33
test of non regression on two last values			
ρ_9 VARI_ELGA/V31)	0,02	9.30093E-08	0,001
γ_9 VARI_ELGA/V32)	0,02	7.0377E-04	0,001

Large deformations, comparison with the modelization B

Variable	Times (s)	Reference	Tolerance
E_{zz} EPSG_ELGA	0,2	0.22385	0,002
σ_{zz} (Mpa) SIEF_ELGA	0,2	320.153	0,09
ρ_1 VARI_ELGA/V7)	0,2	1.731E-05	0,18
γ_1 VARI_ELGA/V8)	0,2	0.31346	0,06
ρ_9 VARI_ELGA/V31)	0,2	8.37E-07	0,06
γ_9 VARI_ELGA/V32)	0,2	0.010410	0,06
ρ_{12} VARI_ELGA/V40)	0,2	1.719E-05	0,24
γ_{12} VARI_ELGA/V41)	0,2	0.11118	0,21
test of non regression			
σ_{zz} (Mpa) SIEF_ELGA	0,2	293.247	0,001
ρ_1 VARI_ELGA/V7)	0,2	1.425E-05	0,001
γ_1 VARI_ELGA/V8)	0,2	0.297258	0,001
ρ_9 VARI_ELGA/V31)	0,2	7.87472E-07	0,001
γ_9 VARI_ELGA/V32)	0,2	9.79517E-03	0,001
ρ_{12} VARI_ELGA/V40)	0,2	1.309E-05	0,001
γ_{12} VARI_ELGA/V41)	the 0,2	0.088585	0,001

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

8 Summary of the results

the results are satisfactory and validate the large deformations of behavior MONOCRISTAL.