SSND110 – Validation of the single-crystal models resulting from the Dynamics of Dislocations

Summarized:

One carries out, on a problem reduced to the material point, a validation of the single-crystal models, either compared to an analytical solution, or with an experimental reference. In the first case (modelizations A and B and C), a monocrystal is charged according to a particular directional sense, allowing the privileged sliding of only one system, at least at the beginning of the loading. In the second case (modelization C), one refers to experimental results quoted by Julien Schwartz in his thesis, which results in simulating a traction test on a polycrystal made up of 40 monocrystals whose behavior is MONO_DD_FAT.

Modelization a: this modelization makes it possible to validate behavior MONO_DD_CFC with SIMU_POINT_MAT.
Modelization b: this modelization makes it possible to validate behavior MONO_DD_CC with SIMU_POINT_MAT.
Modelization C: this modelization makes it possible to validate behavior MONO_DD_FAT with SIMU_POINT_MAT.
Modelization D: this modelization makes it possible to validate behavior MONO_DD_CC_IRRA with SIMU_POINT_MAT.
Modelization E: this modelization makes it possible to validate behavior MONO_DD_CFC_IRRA with SIMU_POINT_MAT.

1 Problem of reference

1.1 Geometry

It acts of a material point, representative of a stress state and strains homogeneous.

1.2 Properties of the materials

1.2.1 Properties for the modelization A, crystalline model MONO_DD_CFC

1.2.1.1 Coefficients relating to isotropic elasticity

Shear modulus: $\mu = 80000.MPa$, Poisson's ratio $\nu = 0.3$
Modulus Young: $E = \mu * 2 * (1. + \nu)$

1.2.1.2 Coefficients of model MONO_DD_CFC

$A = 0.13 \quad B = 0.005 \quad \alpha = 0.35 \quad \beta = 2.5410^{-7} (2.54\ Angström)$
$Y = 2.5 \quad 10^{-7} mm (2.5\ Angstrom) \quad \tau_f = 20. \quad n = 5. \quad \dot{\gamma}_0 = 10^{-3} \quad \rho_{ref} = 10^6\ mm^{-2}$

the matrix of interaction is only made up of 1: $H1 = H2 = H3 = H4 = H5 = 1.0$,
The family of sliding systems is octahedral (CFC).
The local variables representing the density of dislocations are initialized with $\rho_0 * b^2$
$\rho_0 = 10^5\ mm^{-2}$

1.2.2 Properties for the modelization B, crystalline model MONO_DD_CC

1.2.2.1 Coefficients relating to isotropic elasticity

Poisson's ratio $\nu = 0.35$
Modulus Young: $E = (236 - 0{,}0459\ T)$ GPa

1.2.2.2 Coefficients of model MONO_DD_CC

Two sets of coefficients are used according to the cases:

Cases 1 (formulation 1)	Case 2 (formulation 2)
DELTA1 = 0 (formulation 1) TEMP = 300 K D_LAT = 1000 mm K_BOLTZ = 8.62 10^{-5} GAMMA0 = $10^{-3}\ s^{-1}$ TAU_0 = 363 MPa TAU_F = 20 MPa RHO_MOB = 10^5 mm^{-2} K_F = 30 K_SELF = 100 B = 2.48 10^{-7} mm N = 20 DELTAG0 = 0.84 BETA = 0.2 D = 10^{-5} mm GH = 10^{11} Y_AT = 10^{-6} mm , the local variables representing the density of dislocations are initialized with $\rho_0 = 10^5\ mm^{-2}$	DELTA1 = 1 (formulation 2) TEMP = 50 K D_LAT = 1000 mm K_BOLTZ = 8.62 10^{-5} GAMMA0 = $10^{-6}\ s^{-1}$ TAU_0 = 363 MPa TAU_F = 0 RHO_MOB = 10^5 mm^{-2} K_F = 75 K_SELF = 100 B = 2.48 10^{-7} mm N = 50 DELTAG0 = 0.84 BETA = 0.2 D = 10^{-5} mm GH = 10^{11} Y_AT = 2 10^{-6} mm , the local variables representing the density of dislocations are initialized with $\rho_0 = 10^5\ mm^{-2}$, except for the principal system (number 5): $\rho_0 = 10^6\ mm^{-2}$

The matrix of interaction is built in both cases starting from the following values
H1 = 0.1024 , H2 = 0.7 , H3=H4=H5=H6 = 0.1

the family of sliding systems is cubic (CC).

1.2.3 Properties for the modelization C

1.2.3.1 Coefficients relating to orthotropic elasticity

elasticity orthotropic cubic, therefore is defined here by 3 coefficients:

$$y_{1111} = 244000.\ MPa$$
$$y_{1122} = 96000.\ MPa$$
$$y_{1212} = 74000.\ MPa$$

One has then:

$$\nu_{LT} = \nu_{TN} = \nu_{LN} = \nu = \frac{1}{(1+\frac{y_{1111}}{y_{1122}})}$$
$$E_L = E_T = E_N = y_{1111}\frac{(1-3\nu^2-2\nu^3)}{(1-\nu^2)}$$
$$G_{LT} = G_{TN} = G_{LN} = y_{1212}$$

1.2.3.2 Coefficients of model MONO_DD_FAT

$$\tau_f = 44.9\ MPa$$
$$\dot{\gamma}_0 = 4.\ 10^{-11}\ s^{-1}$$
$$\beta = 2.5410^{-7}\ mm\ (2.54\ Angström)$$
$$n = 73.5$$
$$\text{UN\_SUR\_D} = 0.$$
$$g_{c0} = 1.33\ 10^{-6}\ mm$$
$$K = 37.14$$

the matrix of interaction is characterized by the five following coefficients (cf [R5.03.11]):

$$H1 = 0.1236$$
$$H2 = 0.633$$
$$H3 = 0.1388$$
$$H4 = 0.1236$$
$$H5 = 0.0709$$

The family of sliding systems is octahedral.

The local variables representing the density of dislocations are initialized with $\rho_0 \times b^2$
$\rho_0 = 1.77\ 10^6\ mm^{-2}$

1.2.4 Properties for the modelization D, crystalline model MONO_DD_CC_IRRA

1.2.4.1 Coefficients relating to isotropic elasticity

Poisson's ratio $\nu = 0.35$
Modulus Young: $E = (236 - 0{,}0459\ T)$ GPa

1.2.4.2 Coefficients of model MONO_DD_CC_IRRA

$\text{DELTA1} = 0$ (formulation 1) $\text{TEMP} = 250\ K$

$D\_LAT = 1000\,mm$ $K\_BOLTZ = 8.62\ 10^{-5}$
$GAMMA0 = 10^{-3}\,s^{-1}$ $TAU\_0 = 363\,MPa$
$TAU\_F = 20\,MPa$ $RHO\_MOB = 10^{5}\ mm^{-2}$
$K\_F = 30$ $K\_SELF = 100$ $B = 2.48\ 10^{-7} mm$
$N = 20$ $DELTAG0 = 0.84$ $BETA = 0.2$
$D = 10^{-5} mm$ $GH = 10^{11}$ $Y\_AT = 10^{-6} mm$,
$A\_IRRA = 0.3$, $XI\_IRRA = 4.0$, $DELTA2 = 0$
the local variables representing the density of dislocations are initialized with $\rho_0 = 10^5 mm^{-2}$

the matrix of interaction is built 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 cubic (CC).

1.2.5 Properties for the modelization E, crystalline model MONO_DD_CFC_IRRA

1.2.5.1 Coefficients relating to isotropic elasticity

Shear modulus: $\mu = 80000.\,MPa$, Poisson's ratio $\nu = 0.3$
Modulus Young: $E = \mu * 2 * (1. + \nu)$

1.2.5.2 Coefficients of model MONO_DD_CFC

$A = 0.13$ $B = 0.005$ $\alpha = 0.35$ $\beta = 2.5410^{-7} (2.54\ Angström)$
$Y = 2.5\ \ 10^{-7} mm\,(2.5\ Angstrom)$ $\tau_f = 20.$ $n = 5.$ $\dot{\gamma}_0 = 10^{-3}$ $\rho_{ref} = 10^6\, mm^{-2}$

$\alpha^{loops} = 0{,}1$ $\varphi^{loops} = 5.9\ \ 10^{-6}$ $\alpha^{voids} = 0$ $\rho^{voids} = 1.e3$
$\rho_{sat} = 0$ $\varphi_{sat} = 0.04$ $\xi_{irra} = 10$ $\zeta_{irra} = 10^7$ with $\rho_0 = 10^5 mm^{-2}$

the matrix of interaction is characterized by the five following coefficients (cf [R5.03.11]):
$H1 = 0.124$
$H2 = 0.625$
$H3 = 0.137$
$H4 = 0.122$
$H5 = 0.07$
,
the family of sliding systems is octahedral (CFC).
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: $\rho_s^{loops} = 7.4\ \ 10^{-13}\, b^2$
$\phi_s^{voids} = 0.001$

1.3 Boundary conditions and loadings

1.3.1 Loading for the modelizations A, B (case 1), and D

the loading is in imposed stresses:

$$\sigma = \sigma_0\, \mathbf{n} \otimes \mathbf{n}$$

with $\sigma_0 = 100\,MPa$ and $\mathbf{n} = (0.09667365, 0.48336824, 0.87006284)^T$

From where components of the tensor of the stresses imposed:

$\sigma_{xx}=0.93457943925233633$
$\sigma_{yy}=23.364485981308412$
$\sigma_{zz}=75.700934579439235$
$\sigma_{xy}=4.6728971962616823$
$\sigma_{xz}=8.411214953271027$
$\sigma_{yz}=42.056074766355138$

1.3.2 Loading for the modelization B (case 2)

the loading is in imposed strains:

$dt\ \epsilon_{\text{zz imposée}}=3\,10^{-4}\,s^{-1}$ and $\varepsilon_{zz}(tmax)=0,27$ with $tmax=900\,s$

the monocrystal has as a directional sense [- 1,4,9].

1.3.3 Loading for the modelization C

the loading is in imposed strains:

$\epsilon_{\text{zz imposée}}=0.001\,t$ of $t=0\,s$ with $t=45\,s$

1.3.4 Loading for the modelization E

the loading is in imposed strains:

$\epsilon_{\text{zz imposée}}=0.05\,t$ of $t=0\,s$ with $t=1\,s$

1.4 Forced

Initial conditions and null strains.

2 Reference solution

2.1 Reference solution for the modelization A

It leans on [bib.1] and [R5.03.11]. One finds a solution analytical under the assumptions:

- the tensor of the stresses $\boldsymbol{\sigma}$ is known (stresses imposed on a material point)
- the matrix of interaction a_{ij} is only made up of 1.

For each system of sliding, the solved scission is calculated by: $\tau_s = \boldsymbol{\sigma} : \mathbf{m_s}$

with $\mathbf{m_s}$ 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:

$\dot{\gamma}_s = \dot{p}_s \frac{\tau_s}{|\tau_s|}$ where $\dot{p}_s = \dot{\gamma}_0 \left(\left(\frac{|\tau_s|}{\tau_f + \tau_s^{forest}} \right)^n - 1 \right)$ if $|\tau_s| \geq \tau_0 + \tau_s^f$, if not $\dot{p}_s = 0$

with $\tau_s^{forest}(\boldsymbol{\omega}) = \mu\, C(\boldsymbol{\omega}) \sqrt{\sum_{j=1,12} a_{sj} \langle \omega_j \rangle}$ where ω_s is connected to the density of dislocation ρ_s by: : $\omega_s = b^2 * \rho_s$. τ_s being known, $\dot{\gamma}_s$ is thus only function of ω_s .

The evolution of ω_s is given by the differential equation: $\dot{\omega}_s = \dot{p}_s h_s(\langle \omega \rangle)$ with

$$h_s(\omega) = \left(A \frac{\sum_{j \in forest(s)} \sqrt{a_{sj} \langle \omega_j \rangle}}{\sum_{j=1,12} \sqrt{a_{sj} \langle \omega_j \rangle}} + B\, C(\omega) \sum_{j \in copla(s)} \sqrt{a_{sj} \langle \omega_j \rangle} - \frac{y}{b} \langle \omega_s \rangle \right)$$

$$C(\omega) = 0.2 + 0.8 \frac{\ln\left(\alpha \sqrt{\sum_{i=1,12} \langle \omega_i \rangle} \right)}{\ln\left(\alpha\, b \sqrt{\rho_{ref}} \right)} .$$

For the directional sense chosen, that is to say $1\text{-}5\text{-}9$, the factors of Schmid, connecting the tensor of the stresses to the various solved scissions τ_s are, for the 12 octahedral systems of CFC [R5.03.11]: $[0.45784855, 0.22892428, 0.22892428, 0.15261618, 0.26707832, 0.11446214, 0.19840104, 0.29760156, 0.4960026, 0.04578486, 0.11446214, 0.16024699]$

It is thus noted that the first system of activated sliding will be number 9 ($\mathrm{A3}$), and the second will be number 1 (either $\mathrm{B4}$). The scissions solved for these two systems are:

- system $\mathrm{A3}$ (number 9): $\tau_s = 49{,}6\ MPa$
- system $\mathrm{B4}$ (number 1): $\tau_s = 45{,}785\ MPa$

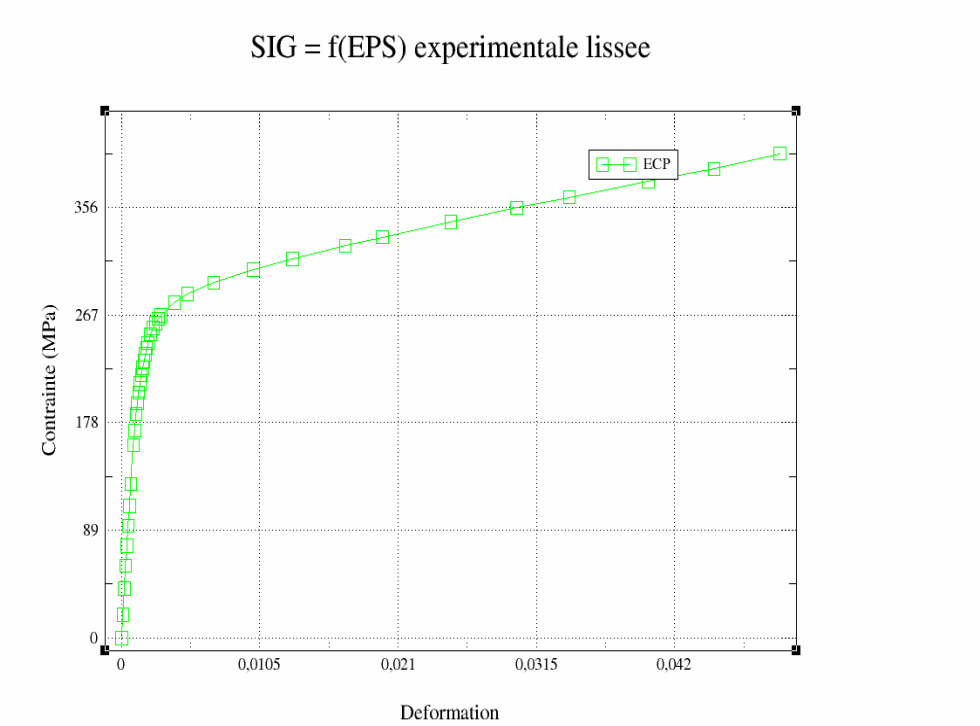
For these two systems, τ_s being known, it is enough to solve the differential equation $\dot{\omega}_s = \dot{p}_s h_s(\langle \omega \rangle)$ to know all the variables. This is carried out numerically, using the modulus “odeint” of scipy (see file `SSND110A.22`).

2.2 Reference solution for the modelization B

In the case of CC , for the directional sense chosen, is $1\text{-}5\text{-}9$, the first system of sliding (CUBIC family) activated will be number 8, and the second will be number 5. The scissions solved for these two systems are:

- system number 8: $\tau_s = 49,6\ Mpa$
- system number 5: $\tau_s = 45,785\ MPa$

2.3 Reference solution for the modelization C



the experimental data are summarized by the curve smoothed below:
For more accuracy, one will be able to refer to [2] and [3].

2.4 Reference solution for the modelization D

the validation consists in checking that sliding systems activated are well those which are expected, and to compare the results between integrations explicit and implicit.

2.5 Reference solution for the modelization E

the validation consists in checking that stress-strain curve obtained with irradiation presents well a on-hardening compared to the case not irradiated, then a softening.

2.6 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] J.M. Stephan Notes EDF-R&D: HT24-2010-01329-FR “Project ANR AFGRAP – monotonous and cyclic Curves of tension average of the steel AISI 316LN (T252 Sheet) provided by AREVA”

[3] J. Schwartz: “Nonlocal Approach in crystalline plasticity: application under investigation of the structural mechanics behavior of steel AISI 316LN in fatigue oligocyclic”. Thesis of the Central School of Paris, June 2011.

[4] G.Monnet: “Hook plasticity constitutive law for irradiated RPV steel” Note EDF R & D HT 27 - 2011 - 02738, December 2011.

3 Modelization A

3.1 Characteristic of the modelization

a material point of behavior DD_CFC, comprising 12 sliding systems (family OCTAEDRIQUE) is requested with imposed stress.

3.2 Quantities tested and Values

3.2.1 results tested

Integration RUNGE_KUTTA

Variable	Times (s)	Variable
ρ_9	1	1
ρ_1	1	1
γ_9	1	1
γ_1	1	1
ε_{xx}^{vp}	1	1
ε_{xx}^{vp}	1	1
ε_{xx}^{vp}	1	1
ε_{xx}^{vp}	1	1

2.807372E-05 IMPLICIT

Integration	Times (s)	Reference
ρ_9	1	7.17405E-09
ρ_1	1	6.60769E-09
γ_9	1	8.003927E-05
γ_1	1	1.72109E-05
ε_{xx}^{vp}	1	-3.9702232E-05
ε_{xx}^{vp}	1	3.970223E-05
ε_{xx}^{vp}	1	1.8136978E-05
ε_{xx}^{vp}	1	2.807372E-05

4 Modelization B

4.1 Characteristic of the modelization

a material point whose single-crystal flow model is MONO_DD_CC, comprising 12 sliding systems of family CUBIQUE1, is requested with imposed stress.

4.2 Quantities tested and Values

4.2.1 results tested

(case 1)

Variable	Times (s)	Reference
ρ_8	1	$1{,}036859\,10^{11}$
ρ_5	1	$1{,}01942\,10^{11}$
γ_8	1	$1{,}9427\,10^{-5}$
γ_5	1	$-1{,}01835\,10^{-5}$
ε_{xx}^{vp}	1	$-1{,}22\,10^{-5}$
ε_{zz}^{vp}	1	$1{,}21\,10^{-5}$
ε_{xx}^{vp}	1	$2{,}6871\,10^{-6}$
ε_{xx}^{vp}	1	$8{,}617\,10^{-6}$

(case 2)

Variable	Times (s)	Reference
ρ_5	100	$3{,}945\,10^{6}$
ρ_5	500	$9{,}087\,10^{6}$
γ_5	100	$-5.44\,10^{-2}$
γ_5	500	$-2.8714\,10^{-1}$

5 Modelization C

5.1 Characteristic of the modelization

a material point whose flow model is that of a polycrystal made up of 40 monocrystals behaving according to model MONO_DD_FAT, comprising 12 sliding systems (family OCTAEDRIQUE), is requested in imposed strain.

5.2 Quantities tested and Values

5.2.1 results tested

Integration RUNGE_KUTTA

Variable	Times (s)	Reference	Aster	Tolerance
σ_{zz}	45	non_regression	424.9353 MPa	0.1%
σ_{zz}	45	source_externe	387.8 MPa	10.0%

6 Modelization D

6.1 Characteristic of the modelization

a material point whose single-crystal flow model is MONO_DD_CC_IRRA, comprising 12 sliding systems of family CUBIQUE1, is requested with imposed stress.

6.2 Quantities tested and Values

6.2.1 results tested

Integration RUNGE_KUTTA

Variable	Times (s)	IMPLICIT
ρ_8	1	$1{,}00044\,10^{11}$
ρ_5	1	$1{,}0002\,10^{11}$
γ_8	1	$2.253361\,10^{-7}$
γ_5	1	$-1.0377\,10^{-7}$
ε_{xx}^{vp}	1	$-1.34842\,10^{-7}$
ε_{zz}^{vp}	1	$1.34505\,10^{-7}$
ε_{xy}^{vp}	1	$3.516926\,10^{-8}$
ε_{yz}^{vp}	1	$9.533983\,10^{-8}$

1 Integration

Comparison to the solution of integration **RUNGE_KUTTA**

Variable	Times (s)	Reference	Tolerance %
ρ_8	1	$1{,}00044\,10^{11}$	0.5
ρ_5	1	$1{,}0002\,10^{11}$	0.1
γ_8	1	$2.253361\,10^{-7}$	0.1
γ_5	1	$-1.0377\,10^{-7}$	2
ε_{xx}^{vp}	1	$-1.34842\,10^{-7}$	0.1
ε_{zz}^{vp}	1	$1.34505\,10^{-7}$	2
ε_{xy}^{vp}	1	$3.516926\,10^{-8}$	2
ε_{yz}^{vp}	1	$9.533983\,10^{-8}$	2

7 Modelization E

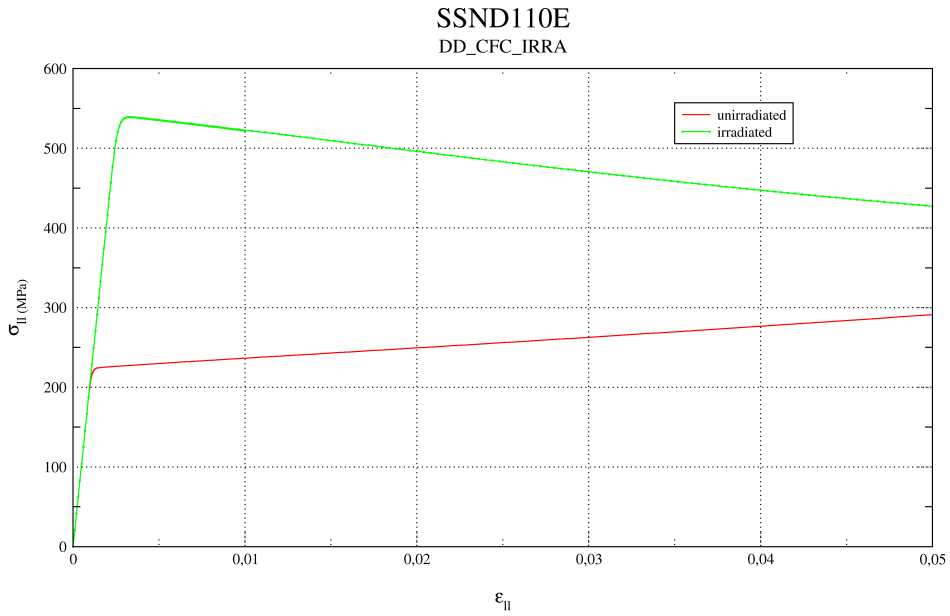
7.1 Characteristic of the modelization

Modelization identical to the modelization A, except the behavior which takes into account the irradiation.

7.2 Quantities tested and Values

7.2.1 results tested

Variable	Times (s)	Reference
σ_{zz}	6,6e-2	539,068
σ_{zz}	1	427,1665
ε_{xx}^{vp}	1	-0,045111
ε_{xx}^{vp}	1	0,047946
ε_{xx}^{vp}	1	0,01472
ε_{xx}^{vp}	1	-5,6913e-3



8 Summary of the results

the results are satisfactory and validate behaviors DD_CFC, DD_CC and DD_FAT.