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

Summary:

One carries out, on a problem reduced to the material point, a validation of the single-crystal laws, either compared to an analytical solution, or with an experimental reference.

For all modelings (except C), one tests monocrystal charged according to a particular orientation, allowing the privileged slip of only one system, at least at the beginning of the loading.

For modeling C, one refers to experimental results quoted by Julien Schwartz in his thesis, which results in simulating a tensile test on a polycrystal made up of 40 monocrystals whose behavior is MONO_DD_FAT.

Modeling a: this modeling makes it possible to validate the behavior MONO_DD_CFC
Modeling b: this modeling makes it possible to validate the behavior MONO_DD_CC
Modeling C: this modeling makes it possible to validate the behavior MONO_DD_FAT
Modeling D: this modeling makes it possible to validate the behavior MONO_DD_CC_IRRA
Modeling E: this modeling makes it possible to validate the behavior MONO_DD_CFC_IRRA.

1 Problem of reference

1.1 Geometry

It is about a material point, representative of a stress and strain state homogeneous.

1.2 Properties of materials

1.2.1 Properties for modeling A, crystalline law MONO_DD_CFC

1.2.1.1 Coefficients relating to isotropic elasticity

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

1.2.1.2 Coefficients of the law MONO_DD_CFC

$A = 0.13 \quad B = 0.005 \quad \alpha = 0.35 \quad \beta = 2.5410^{-7} (2.54\ Angström)$
$Y = 2.5 \;\; 10^{-7} mm\,(2.5\ Angstrom) \quad \tau_f = 20. \quad n = 5. \quad \dot{\gamma}_0 = 10^{-3}$
$\rho_{ref} = \rho_{tot} = 1.2\,10^{6}\ mm^{-2}$ is initial total density, being used to calculate the matrix of corrected interaction, of which the coefficients evolve with the density of total dislocation.

The matrix of interaction is only made up of 1: $H1 = H2 = H3 = H4 = H5 = 1.0$,
The family of systems of slip is octahedral (CFC) .
Each variable interns representing the density of dislocation of a system of slip is initialized with $\rho_0 * b^2$ with $\rho_0 = 10^5\ mm^{-2} = \frac{\rho_{tot}}{12}$

1.2.2 Properties for modeling B, crystalline law MONO_DD_CC

1.2.2.1 Coefficients relating to isotropic elasticity

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

1.2.2.2 Coefficients of law MONO_DD_CC

Two sets of coefficients are used according to the cases:

Case 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 internal 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 internal 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 systems of slip is cubic (CC).

1.2.3 Properties for modeling 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:

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

Note: the coefficient μ^{loca} used for the localization is worth 74000 Mpa.

1.2.3.2 Coefficients of the law MONO_DD_FAT

$\tau_f=44.9\ MPa$
$\dot{\gamma}_0=4.\ 10^{-11}\ s^{-1}$
$\beta=2.5410^{-7}\ mm\ (2.54\ Angström)$
$n=73.5$
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 systems of slip is octahedral.

The internal variables representing the density of dislocations are initialized with $\rho_0\times b^2$ with $\rho_0=1.7710^6\ mm^{-2}$

1.2.4 Properties for modeling D, crystalline law MONO_DD_CC_IRRA

1.2.4.1 Coefficients relating to isotropic elasticity

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

1.2.4.2 Coefficients of the law MONO_DD_CC_IRRA

$TEMP=250\,K$
$D\_LAT=1000\,\text{mm}$ $K\_BOLTZ=8.62\ 10^{-5}$
$GAMMA0=10^{-3}\,s^{-1}$ $TAU\_0=363\,\text{MPa}$
$TAU\_F=20\,\text{MPa}$
$K\_F=30$ $K\_SELF=100$ $B=2.48\ 10^{-7}\,\text{mm}$
$N=20$ $DELTAG0=0.84$
$D=10^{-5}\,\text{mm}$ $GH=10^{11}$, $Y\_AT=10^{-6}\,\text{mm}$,
$A\_IRRA=0.3$, $XI\_IRRA=4.0$,

The internal variables representing the density of dislocations are initialized with $\rho_0=10^5\,mm^{-2}=\frac{\rho_{tot}}{12}$ with $\rho_{tot}=1{,}2\,10^6\,mm^{-2}$

$RHO\_MOB=\rho_0$ has mobile density by system of slip.

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 systems of slip is cubic (CC).

1.2.5 Properties for modeling E, crystalline law MONO_DD_CFC_IRRA

1.2.5.1 Coefficients relating to isotropic elasticity

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

1.2.5.2 Coefficients of the law MONO_DD_CFC

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

$\alpha^{loops}=0{,}1$ $\varphi^{loops}=5.9\ \ 10^{-6}$ $\alpha^{voids}=0$ $\rho^{voids}=1.e3$
$\rho_{sat}=0$ $\varphi_{sat}=0.04$ $\xi_{irra}=10$ $\zeta_{irra}=10^7$ with $\rho_0=\frac{10^5}{12}\,mm^{-2}$

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 systems of slip is octahedral (CFC) .
The internal variables representing the density of dislocations are initialized with ρ_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 modelings A, B (case 1), and D

The loading is in imposed constraints:

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

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

From where components of the tensor of the constraints 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 modeling B (case 2)

The loading is in imposed deformations:

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

The monocrystal has as an orientation [- 1,4,9].

1.3.3 Loading for modeling C

The loading is in imposed deformations:

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

1.3.4 Loading for modeling E

The loading is in imposed deformations:

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

1.4 Initial conditions

Worthless constraints and deformations.

2 Reference solution

2.1 Reference solution for modeling A

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

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

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

with $\mathbf{m_s}$ 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:

$\dot{\gamma}_s = \dot{p}_s \frac{\tau_s}{|\tau_s|}$ 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 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 .

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 orientation chosen, that is to say $1\text{-}5\text{-}9$, factors of Schmid, connecting the tensor of the constraints 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 slip 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): $\tau_s = 45{,}785\ MPa$

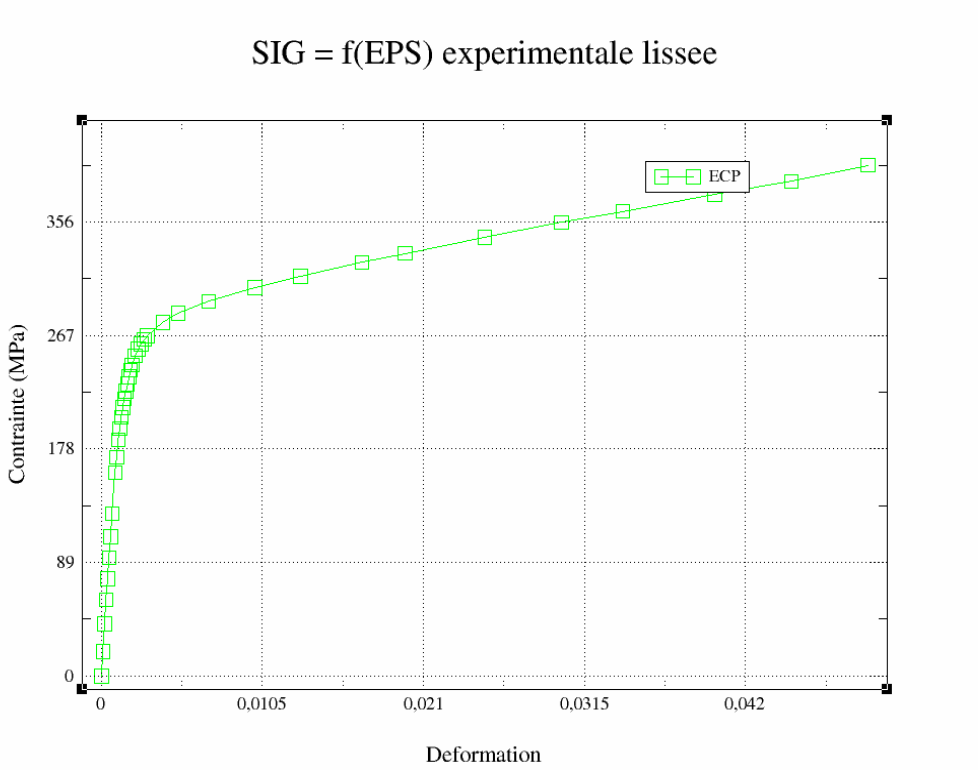
For these two systems, τ_s being known, it is enough to solve the differential equation $\dot{\omega}_s = \dot{p}_s h_s(\langle \omega \rangle)$ to know the whole of the variables. This is carried out numerically, using the module "odeint" of scipy (see file `SSND110A.22`).

2.2 Reference solution for modeling B

In the case of it CC , for the orientation chosen, that is to say $1\text{-}5\text{-}9$, the first system of slip (CUBIC family) activated will be number 8, and the second will be number 5. The scissions solved for these two systems are (at a temperature of 300K):

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

2.3 Reference solution for modeling C



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

2.4 Reference solution for modeling D

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

2.5 Reference solution for modeling E

The validation consists in checking that stress-strain curve obtained with irradiation presents well a on-work 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 Note EDF-R&D: HT24-2010-01329-FR “Project ANR AFGRAP – monotonous and cyclic Diagrams traction average of the steel AISI 316LN (T252 Sheet) provided by AREVA”

[3] J. Schwartz: “Nonlocal approach in crystalline plasticity: application under investigation of the mechanical 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 Modeling A

3.1 Characteristics of modeling

A material point of behavior DD_CFC, comprising 12 systems of slip (family OCTAHEDRAL) is solicited with imposed constraint.

3.2 Sizes tested and results

3.2.1 Values tested

Integration RUNGE_KUTTA

Variable	Moments (s)	Reference	Tolerance %
ρ_9	1	7.17E-09	0.1
ρ_1	1	6.608E-09	0.1
γ_9	1	8.00E-05	0.1
γ_1	1	1.72E-05	0.2
ε_{xx}^{vp}	1	-3.97E-05	0.1
ε_{xx}^{vp}	1	3.97E-05	0.1
ε_{xx}^{vp}	1	1.81E-05	0.1
ε_{xx}^{vp}	1	2.81E-05	0.1

Integration IMPLICIT

Variable	Moments (s)	Reference	Tolerance %
ρ_9	1	7.17E-09	0.5
ρ_1	1	6.608E-09	0.1
γ_9	1	8.00E-05	1
γ_1	1	1.72E-05	2
ε_{xx}^{vp}	1	-3.97E-05	1
ε_{xx}^{vp}	1	3.97E-05	1
ε_{xx}^{vp}	1	1.81E-05	1
ε_{xx}^{vp}	1	2.81E-05	1

4 Modeling B

4.1 Characteristics of modeling

A material point whose single-crystal law of flow is MONO_DD_CC, comprising 12 systems of slip of the family CUBIQUE1, is solicited with imposed constraint.

4.2 Sizes tested and results

4.2.1 Values tested

Temperature 300K

Variable	Moments (s)	Reference
τ_8	1	$4{,}96\,10^{7}$
τ_5	1	$-4{,}57810^{7}$
ρ_8	1	$1{,}0215210^{11}$
ρ_5	1	$1{,}0113910^{11}$
γ_8	1	$2{,}1173\,10^{-5}$
γ_5	1	$-1{,}10927\,10^{-5}$
ε_{xx}^{vp}	1	$-1{,}3283\,10^{-5}$
ε_{zz}^{vp}	1	$1{,}3216\,10^{-5}$
ε_{xy}^{vp}	1	$2{,}9309\,10^{-6}$
ε_{yz}^{vp}	1	$9{,}3901\,10^{-6}$

Temperature 50K

Variable	Moments (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 Modeling C

5.1 Characteristics of modeling

A material point whose law of flow is that of a polycrystal made up of 40 monocrystals behaving according to the law MONO_DD_FAT, comprising 12 systems of slip (family OCTAHEDRAL), is solicited in imposed deformation.

5.2 Sizes tested and results

5.2.1 Values tested

Integration RUNGE_KUTTA

Variable	Moments (s)	Reference	Aster	Tolerance
σ_{zz}	45	non_regression	407.71 MPa	0.1%
σ_{zz}	45	source_externe	387.8 MPa	6.0%

6 Modeling D

6.1 Characteristics of modeling

A material point whose single-crystal law of flow is MONO_DD_CC_IRRA, comprising 12 systems of slip of the family CUBIQUE1, is solicited with imposed constraint.

6.2 Sizes tested and results

6.2.1 Values tested

Integration RUNGE_KUTTA

Variable	Moments (s)	Reference
ρ_8	1	1.0003807E+11
ρ_5	1	1.0001773E+11
γ_8	1	2.470697430610E-07
γ_5	1	-1.139016265372E-07
ε_{xx}^{vp}	1	-1.479102030578E-07
ε_{zz}^{vp}	1	1.475432149480E-07
ε_{xy}^{vp}	1	3.852669669294E-08
ε_{yz}^{vp}	1	1.045760539705E-07

Integration IMPLICIT
(comparison with integration clarifies)

Variable	Moments (s)	Reference	Tolerance %
ρ_8	1	1.0003807E+11	0.5
ρ_5	1	1.0001773E+11	0.5
γ_8	1	2.470697430610E-07	2
γ_5	1	-1.139016265372E-07	2
ε_{xx}^{vp}	1	-1.479102030578E-07	5
ε_{zz}^{vp}	1	1.475432149480E-07	2
ε_{xy}^{vp}	1	3.852669669294E-08	2
ε_{yz}^{vp}	1	1.045760539705E-07	2

Note: the variations are due to the discretization in time, coarser with implicit integration.

7 Modeling E

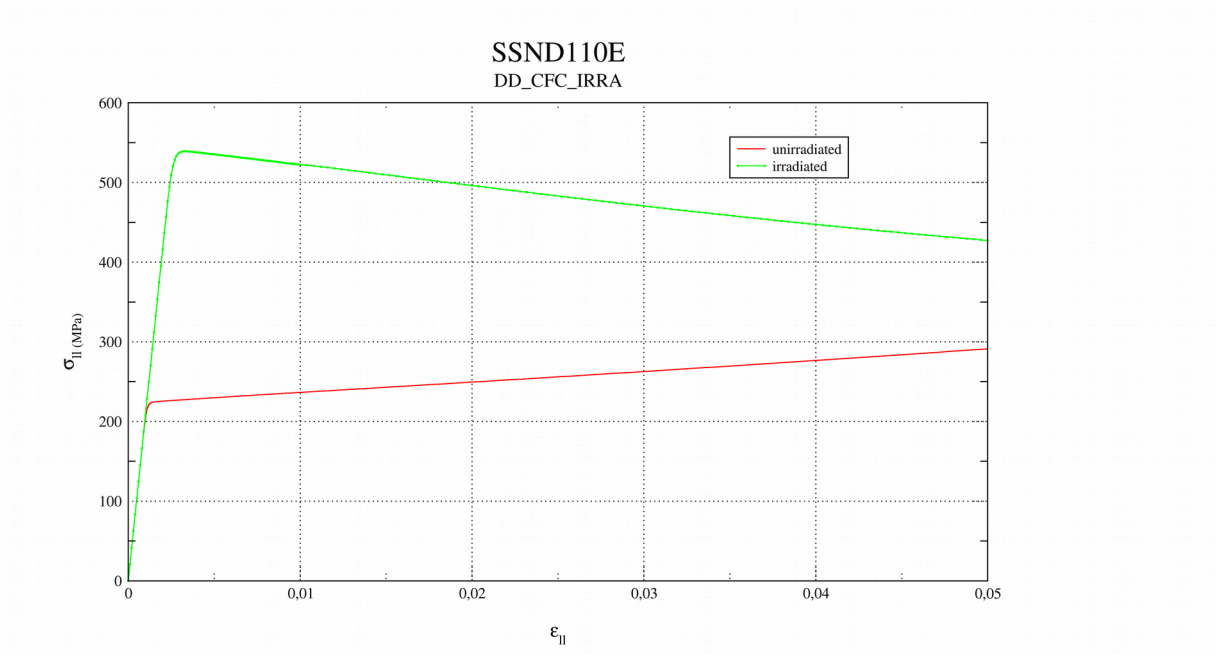
7.1 Characteristics of modeling

Modeling identical to modeling A, except the behavior which takes into account the irradiation.

7.2 Sizes tested and results

7.2.1 Values tested

Variable	Moments (s)	Reference	Tolerance %
σ_{zz}	6,6e-2	539.068	0.2
σ_{zz}	1	427.1665	2
ε_{xx}^{vp}	1	-0.045111	0.1
ε_{xx}^{vp}	1	0.047946	0.1
ε_{xx}^{vp}	1	0.01472	0.3
ε_{xx}^{vp}	1	-5,6913e-3	0.1



8 Summary of the results

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