MFRON03 – Test of the interface *Code_Aster-MFront* for crystalline laws

Summary:

This test validates behaviors orthotropic defined using *MFront* by comparison with similar behaviors of *Code_Aster*.

Modeling b: this modeling makes it possible to validate the model single-crystal élasto-visco-plastic with implicit integration, by comparison with the model MONOCRYSTAL on a material point.

Modeling C: this modeling makes it possible to validate the model single-crystal élasto-visco-plastic with implicit integration, and complete definition of the family of systems of slip and the matrix of interaction, by comparison with the model MONOCRYSTAL of Code_Aster on an aggregate with 10 grains.

Modeling D: this modeling makes it possible to validate the model polycrystalline élasto-visco-plastic with explicit integration, by comparison with the model POLYCRYSTAL on a material point with 30 grains.

Modeling E: this modeling makes it possible to validate the model single-crystal élasto-visco-plastic of type `DD_CFC` on a material point.

Modeling F: this modeling makes it possible to validate the model polycrystalline élasto-visco-plastic homogenized of type `DD_CFC` on a material point with 30 grains.

Modeling G: this modeling makes it possible to validate the model single-crystal élasto-visco-plastic of type `DD_CFC_IRRA` on a material point.

Modeling H: this modeling makes it possible to validate the model single-crystal élasto-visco-plastic homogenized of type `DD_CC` on a material point.

Modeling I: this modeling makes it possible to validate the model single-crystal élasto-visco-plastic of type `DD_CC_IRRA` on a material point.

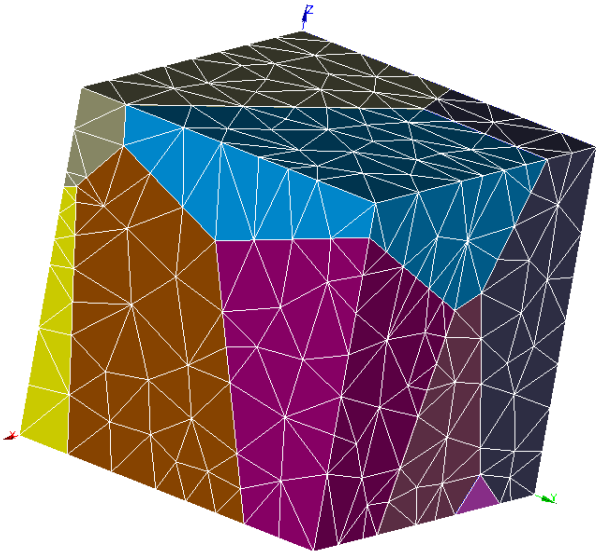
Modeling J: this modeling makes it possible to validate the model single-crystal élasto-visco-plastic in great deformations.

Modeling K: this modeling makes it possible to validate the model élasto-visco-plastic polycrystalline homogenized of type `DD_CC` on a material point with 30 grains.

1 Problem of reference

1.1 Geometry

The geometry of modeling C is that of an aggregate with 10 grains generated by a procedure python based on cells of Voronoï. One defines plans of cut in the edges to impose the boundary conditions.



Other modelings are carried out on material points (SIMU_POINT_MAT).

1.2 Properties of materials

1.2.1 Modeling b: monocrystal

This modeling makes it possible to validate the model single-crystal élasto-visco-plastic with implicit integration, by comparison with the model MONOCRYSTAL on a material point.
The coefficients materials are:

E	208000
NAKED	0.3
G	80000
NR	10
K	25
C	14363
R_0	66.62
Q	11.43
B	2.1
D	494

The Mfront files defining the behavior are:
MonoCrystal_CFC.mfront

1.2.2 Modeling C: monocrystal on an aggregate of 10 grains

This modeling makes it possible to validate the model single-crystal élasto-visco-plastic with implicit integration, and complete definition of the family of systems of slip and the matrix of interaction, by comparison with the model MONOCRYSTAL on an aggregate with 10 grains.
The coefficients materials are:

E	210000
NAKED	0.3
G	80769.23
NR	12
K	5
C	0
R_0	250
Q	55
B	12
D	0

The Mfront files defining the behavior are:

MonoCrystal_CFC.mfront

1.2.3 Modeling D: polycrystal homogenized on 30 grains

This modeling makes it possible to validate the model polycrystalline élasto-visco-plastic with explicit integration, by comparison with the model POLYCRYSTAL on a material point with 30 grains. The coefficients materials are:

E	145200
NAKED	0.3
G	55846.15
NR	10
K	40
C	0
R_0	75.5
Q	9.77
B	19.34
D	0

The Mfront files defining the behavior are:

PolyCrystal_MC.mfront
PolyCrystal_Orientation.mfront

The file " PolyCrystal_Orientation.mfront " defines 30 triplets of angles of Euler in degrees.

1.2.4 Modeling E: monocrystal DD_CFC

This modeling makes it possible to validate single-crystal model DD_CFC on a material point, by comparison with MONO_DD_CFC. The coefficients materials are:

E	208000
NAKED	0.3
G	80000
TAU_F	105
Y	2.5E-7
NR	5
GAMMA_0	1.E-3
With	0.13
B	0.005
RHOREF	1.E6
ALPHA	0.35
BETA	2,54E-7
G	80000

The density of initial dislocation is worth 1.E6. The analytical solution is contained in the file mfron03e.30. The Mfront files defining the behavior are:
MonoCrystalDDCFC.mfront
MonoCrystal_DD_CFC_InteractionMatrix.mfront

1.2.5 Modeling F: homogenized polycrystal of type DD_CFC on 30 grains

This modeling makes it possible to validate the homogenized polycrystalline model DD_CFC on a material point with 30 grains, by comparison with POLYCRYSTAL. The coefficients materials are:

E	208000
NAKED	0.3
G	80000
TAU_F	80
Y	2.5E-7
NR	20
GAMMA_0	1.E-3
With	0.13
B	0.005
RHOREF	1.E6
ALPHA	0.35
BETA	2,54E-7
G	80000

The density of initial dislocation is worth 1.E5. The Mfront files defining the behavior are:
PolyCrystalDDCFC.mfront
MonoCrystal_DD_CFC_InteractionMatrix.mfront
The file " PolyCrystal_Orientation.mfront " defines 30 triplets of angles of Euler in degrees.

1.2.6 Modeling G: monocrystal DD_CFC_IRRA

This modeling makes it possible to validate the model DD_CFC_IRRA on a material point, by comparison with the behavior MONO_DD_CFC_IRRA. The coefficients materials are:

E	208000
NAKED	0.3
G	80000
TAU_F	80
Y	2.5E-7
NR	20
GAMMA_0	1.E-3
With	0.13
B	0.005
RHOREF	1.E6
ALPHA	0.35
BETA	2,54E-7
G	80000
ome_void	1000,
PHI_LOOP	5,9E-6
ALP_VOID	0
ALP_LOOP	0.1
ome_sat	0
PHI_SAT	4, E-2
XI_IRRA	10
DZ_IRRA	1, E7

The initial internal variables are:
RHO_0=1, E5
RHO_LOOPS=7,4E13
PHI_VOIDS=1.e-3

The Mfront files defining the behavior are:
MonoDDCFC_Irra.mfront
MonoCrystal_DD_CFC_InteractionMatrix.mfront

1.2.7 Modeling H: monocrystal DD_CC

This modeling makes it possible to validate the model DD_CC on a material point, by comparison with the behavior MONO_DD_CC test ssnd110b. The coefficients materials are:

E (GPa)	236-0.0459*TEMP

NAKED	0.35
G	80000
B	2,48e-7
GH	1.e11
DeltaG0	0.84
TAU_0 (MPa)	363
TAU_F	0
gamma0	1, e-6
N	50
rho_ini	1, e5*B ** 2
D	1.e-5
d_lat	1000.
y_at	2.e-6
K_f	30,
K_self	100
k_boltz	8.62E-5
epsi_1	3rd-4
G	80000
a_self	0.1024
a_coli	0.7
a_ncol	0.1

The temperature of simulation is worth 50 K.

The density of initial dislocation is worth 1.E5 (multiplied by BETA ** 2).

The Mfront files defining the behavior are:

```
MonoCrystalDDCC.mfront
MonoCrystal_DD_CC_InteractionMatrix.mfront
MonoCrystal_DD_CC_SlidingSystems.mfront
```

The monocrystal is defined according to the orientation -1,4,9. It is subjected to an imposed deformation ε_{zz} .

1.2.8 Modeling I: monocrystal DD_CC_IRRA

This modeling makes it possible to validate the model DD_CC_IRRA on a material point, by comparison with the behavior MONO_DD_CC_IRRA test ssnd110d. The coefficients materials are:

E (GPa)	236-0.0459*TEMP
NAKED	0.35
G	80000
B	2,48e-7
GH	1.e11
DeltaG0	0.84

TAU_0 (MPa)	363
TAU_F	20
gamma0	1, e-3
N	20
rho_ini	1, e5*B ** 2
D	1.e-5
d_lat	1000.
y_at	1.e-6
K_f	30,
K_self	100
k_boltz	8.62E-5
epsi_1	1e-5
G	80000
a_irr	0.3
xi_irr	4
a_self	0.1024
a_coli	0.7
a_ncol	0.1

The temperature of simulation is worth 250 K.
The monocrystal is subjected to a traction imposed according to orientation 1,5,9
Density of initial dislocation 1.E5 is worth (multiplied by BETA ** 2). The Mfront files defining the behavior are:
MonoDDCC_Irra.mfront
MonoCrystal_DD_CC_InteractionMatrix.mfront
MonoCrystal_DD_CC_SlidingSystems.mfront

1.2.9 Modeling J: monocrystal in great deformation

This modeling makes it possible to validate the single-crystal model in great deformation on a material point, by comparison with the behavior MONOCRYSTAL test ssnd112a. The coefficients materials are:

N	10.
K	25.0
C	14363.
R_0	66.62
Q	11.43
B	2.1
D	494.
H1	1.
H2	1.
H3	0.6
H4	12.3
H5	1.6
H6	1.8

The Mfront files defining the behavior are:
GdefMonoCrystal.mfront
GdefMono_Jacnum.mfront

1.2.10 Modeling K: homogenized polycrystal DD_CC

This modeling makes it possible to validate the homogenized polycrystalline model DD_CC on a material point with 30 grains, by comparison with the behavior POLYCRYSTAL test ssnv194d. The coefficients materials are:

E (GPa)	236-0.0459*TEMP
NAKED	0.35
G	80000
B	2,48e-7
GH	1.e11
DeltaG0	0.84
TAU_0 (MPa)	363
TAU_F	0
gamma0	1, e-6
N	50
rho_ini	1, e5*B ** 2
D	1.e-5
d_lat	1000.
y_at	2.e-6
K_f	30,
K_self	100

k_boltz	8.62E-5
epsi_1	3rd-4
G	80000
a_self	0.1024
a_coli	0.7
a_ncol	0.1

The Mfront files defining the behavior are:
PolyCrystalDDCC.mfront
PolyCrystal_DD_CC_SlidingSystems.mfront
MonoCrystal_DD_CC_InteractionMatrix.mfront

2 Reference solution

Values of the constraints, deformations and variables internal, by intercomparison between each behavior Mfront and the behavior are equivalent of Code_Aster.

3 Modeling B

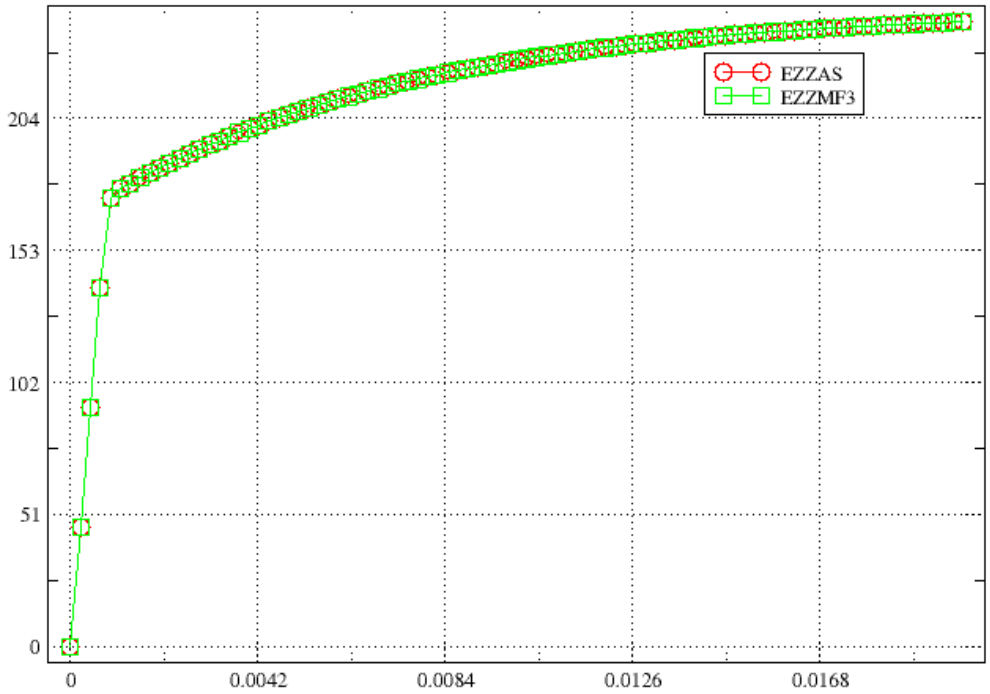
3.1 Characteristics of modeling

Not material. SINGLE-CRYSTAL behavior. The law tested is MonoCrystal_CFC.mfront

3.2 Grandeurs tested and results

One compares the solution obtained with the behavior MonoCrystal_CFC de Mfront and that obtained with the behavior MONOCRYSTAL of Code_Aster, by testing the maximum of relative difference of the following components:

Component	Moment (S)	Reference (difference)	Absolute tolerance
SIZZ	Maximum change	0	1.E-6
Rho_1*beta ** 2	Maximum change	0	1.E-5



Forced curves SIZZ according to deformations EPZZ for MFRONT and CODE_ASTER for the behavior CFC MONOCRYSTAL.

4 Modeling C

4.1 Characteristics of modeling

Many nodes: 552.
Modeling 3D : 2269 tetrahedral elements of volume: TETRA4.
The families of systems of slip are of octahedral type. The structure contains 10 grains generated by a procedure in python which bases itself on cells of Voronoï. With each grain corresponds 3 angles of Euler which lay down the directions of the systems of slip.

4.2 Grandeurs tested and results

Comparison between the results got and *Code_Aster* at the calculated last moment.

Identification	Reference	Tolerance %
σ_{xx} of SIEF_ELGA	-16,112	0.01
ε_{xx} of EPSI_ELGA	-1,0250E-03	0.01
ε_{yy} of EPSI_ELGA	-9.3714E-04	0.01
ε_{yy} of EPSP_ELGA	-2 .7745E-04	0.01

5 Modeling D

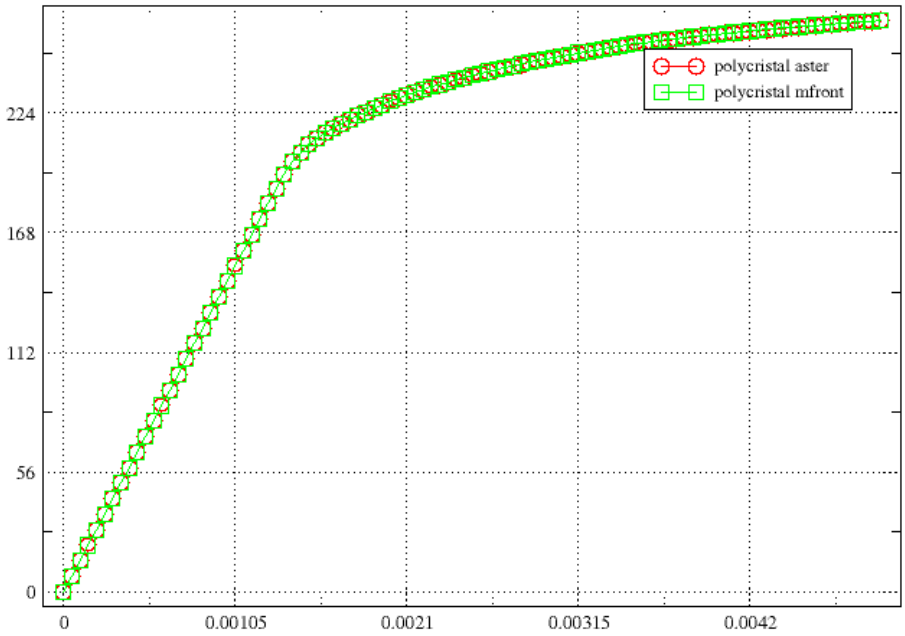
5.1 Characteristics of modeling

Homogenized polycrystalline behavior. On material point. 30 grains of fixed orientations.
The law used is PolyCrystal_MC.mfront

5.2 Grandeurs tested and results

One compares the solution obtained with the Mfront behavior and that obtained with the behavior POLYCRYSTAL, by testing the maximum of relative difference of the following components:

Component		Reference (difference)	Absolute tolerance
SIZZ	Somme of the variations	0	8.77



Forced curves SIZZ according to deformations EPZZ for MFRONT and CODE_ASTER for the behavior POLYCRYSTAL MC.

6 Modeling E

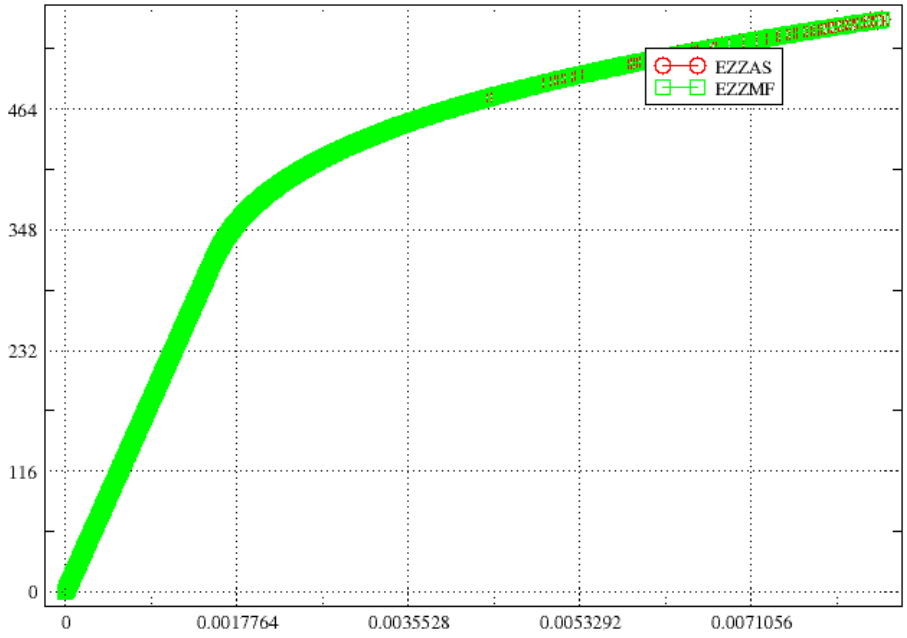
6.1 Characteristics of modeling

Single-crystal behavior DD_CFC. Not material. The law used is MonoCrystalDDCFC.mfront

6.2 Grandeurs tested and results

One compares the solution obtained with the Mfront behavior and that obtained with the behavior MONOCRYSTAL DD_CFC, by testing the maximum of relative difference of the following components:

Component	Moment (S)	Reference (difference)	Absolute tolerance
EPZZ	Maximum change	0	1.E-4
Rho_1*beta ** 2	Maximum change	0	1.E-4



Forced curves SIZZ according to deformations EPZZ for MFRONT and CODE_ASTER for the behavior MONOCRYSTAL DD_CFC.

7 Modeling F

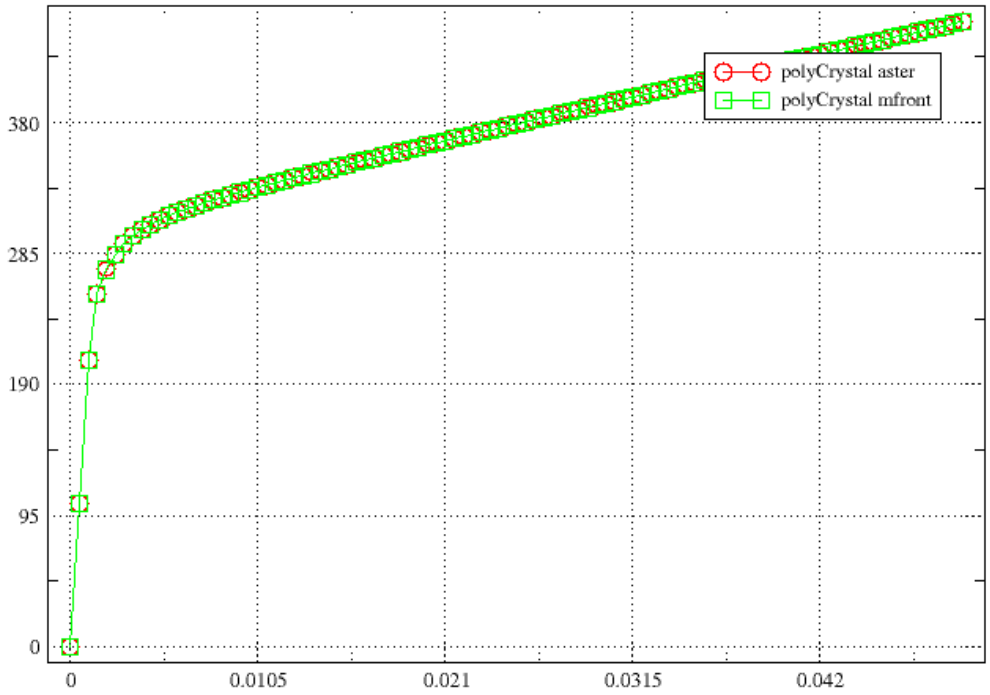
7.1 Characteristics of modeling

Polycrystalline behavior homogenized DD_CFC. Not material. 30 grains of fixed orientations.
The law used is PolyCrystalDDCFC.mfront

7.2 Grandeurs tested and results

One compares the solution obtained with the Mfront behavior and that obtained with the behavior POLYCRYSTAL of the type DD_CFC, by testing the maximum of difference of the following components:

Component	Relative variation	Reference (difference)	Absolute tolerance
SIZZ	Maximum change	0	1.E-3



Forced curves SIZZ according to deformations EPZZ for MFRONT and CODE_ASTER for the behavior POLYCRYSTAL DD_CFC.

8 Modeling G

8.1 Characteristics of modeling

Single-crystal behavior DD_CFC_IRRA. Not material.
The law used is MonoDDCFC_Irra.mfront

8.2 Grandeurs tested and results

One compares the solution obtained with the Mfront behavior and that obtained with the behavior MONO_DD_CFC_IRRA, by testing the maximum of difference of the following components:

Component	Moment (S)	Reference (difference)	Absolute tolerance
SIZZ	Maximum change	0	1.E-8
Rho_1*beta ** 2	Maximum change	0	1.E-8

9 Modeling H

9.1 Characteristics of modeling

Not material. Crystal of orientation (- 1,4,9). Single-crystal behavior DD_CC.

The law used is MonoCrystalDDCC.mfront.

9.2 Grandeurs tested and results

One compares the solution obtained with the Mfront behavior and that obtained with the behavior MONO_DD_CC by testing the maximum of relative difference of the following components:

Component	Moment (S)	Reference (difference)	Tolerance relative
rho_5	Maximum change	0	1.E-3

10 Modeling I

10.1 Characteristics of modeling

Not material. Single-crystal behavior DD_CC_IRRA.

The law used is MonoDDCC_Irra.mfront

10.2 Grandeurs tested and results

One compares the solution obtained with the Mfront behavior and that obtained with the behavior MONO_DD_CC_IRRA by testing the maximum of relative difference of the following components :

Component	Moment (S)	Reference (difference)	Tolerance relative
rho_8	Maximum change	0	1.E-3
rho_5	Maximum change	0	1.E-4

11 Modeling J

11.1 Characteristics of modeling

Single-crystal behavior in great deformations. The laws used are FiniteStrainSingleCrystal.mfront and FiniteStrainSingleCrystal_NumericalJacobian.mfront

Modeling similar to test SSND112A, but with a behavior MONO_VISC1.

11.2 Grandeurs tested and results

One compares the solution obtained with the Mfront behavior and that obtained with the behavior MONOCRYSTAL and DEFORMATION=' SIMO_MIEHE'.

Component	Moment (S)	Reference (aster)	Tolerance relative
ε_{zz}	0.1	0.1066652	0.001
σ_{zz}	0.1	278.978407	0.001
γ_1	0.1	0.18838793	0.003
γ_9	0.1	3.9782E-03	0.08
γ_{12}	0.1	6.184097E-03	0.02

12 Modeling K

12.1 Characteristics of modeling

Not material. 30 grains of fixed orientations. Homogenized polycrystalline behavior DD_CC.
The law used is PolyCrystalDDCC.mfront

12.2 Grandeurs tested and results

One compares the solution obtained with the Mfront behavior and that obtained with the similar behavior POLYCRYSTAL of the type DD_CC, by testing the maximum of relative difference of the following components:

Component	Moment (S)	Reference (difference)	Tolerance
EPZZ	Maximum change	0	1.E-6
SIZZ	Maximum change	0	3.E-2

13 Summary of the results

The results are satisfactory and validate the interface enters *Code_Aster* and MFRONT in 3D, for behaviors with crystalline behaviors.