

## Operator CALC\_META

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### 1 Goal

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Calculate the metallurgical evolution associated with a thermal history.

The operator functions as a postprocessing of the result of thermal calculation in the direction where this last is a data "entering" of metallurgical calculation and which there is not coupling between the metallurgy and it thermal. Two models of evolution are available:

- a model dedicated to the austénite-ferritic transformations of steel,
- a model dedicated to the transformations of zirconium alloys.

Calculation is done with the nodes.

The got result could be used thereafter in data of loading of a mechanical calculation thermo - with taking into account of the metallurgy. One can also at the conclusion of a calculation metallurgy carry out a calculation of postprocessing of hardness.

Réentrant operator, enriches a structure of data `evol_ther`.

## 2 Syntax

```
temper = CALC_META (
    ◇ reuse = temper,
    ◆ MODEL = Mo , [model]
    ◆ CHAM_MATER = chmat , [cham_mater]
    ◇ / ALL = 'YES', [DEFECT]
      / GROUP_MA = lgrma, [l_gr_maille]
    ◆ RESULT = temper, [evol_ther]
    ◆ ETAT_INIT = _F (
        ◆ / META_INIT_ELNO = phasinit, [map]
        / EVOL_THER = temper [evol_ther]
        ◆ / NUME_INIT = nuini_temper, [I]
          / INST_INIT = to, [R]
            ◇ / CRITERION = 'RELATIVE' [DEFECT]
              ◇ PRECISION = / 1.E-6 [DEFECT]
                / prec [R]
            / CRITERION = 'ABSOLUTE'
              ◆ PRECISION = /prec [R]
        ),
    ◆ BEHAVIOR = _F (
        ◆ RELATION = / 'STEEL',
          / 'ZIRC',
    If RELATION = 'STEEL'
    {
        ◇ / LOI_META = 'WAECKEL', [DEFECT]
    }
    If RELATION = 'ZIRC'
    {
        ◇ / LOI_META = 'EDGAR', [DEFECT]
    }
        ◇ / ALL = 'YES', [DEFECT]
          / GROUP_MA = lgrma, [l_gr_maille]
        ),
    ◇ OPTION = | 'DURT_ELNO',
              | 'DURT_NOEU',
              | 'META_ELNO',
              | 'META_NOEU',
    )
)
```

## 3 Operands

### 3.1 Operands MODEL / CHAM\_MATER

- ◆ MODEL = Mo,  
Name of the model whose elements are the object of metallurgical calculation.
- ◆ CHAM\_MATER = chmat,  
Name of the field of affected material on the model Mo.

### 3.2 Operand RESULT

- ◆ RESULT = temper,  
Name of the result `evol_ther` resulting from a thermal calculation from which a metallurgy calculation is done. This result will be at the conclusion of the calculation enriched by the metallurgical evolution of field, internal fields of variables of which the number and the significance depend on the model on transformation used (cf [§3.3.1]).

### 3.3 Selection of the meshes concerned with calculation

Keywords ALL and GROUP\_MA allow the user to choose the meshes on which it wishes to do his elementary calculations of postprocessing.

```
/ ALL = 'YES'
```

All the meshes (carrying finite elements) will be treated. It is the value by default.

```
/ GROUP_MA = l_grma
```

Only meshes included in `l_grma` will be treated.

### 3.4 Keyword BEHAVIOR

- ◆ BEHAVIOR =  
Inform the metallurgical model of evolution used. One can use only one model of evolution per calculation.

#### 3.4.1 Operand RELATION

```
◆ RELATION = / 'STEEL',  
              / 'ZIRC',
```

```
/ 'STEEL'
```

Is used to specify the execution of the calculation of the metallurgical transformations of steel, around  $800^{\circ}C$ , of a ferritic phase (ferrite, pearlite, bainite, martensite) to an austenitic phase (and conversely with cooling). The model with the heating and cooling are different (the selection of this model is done according to the keyword `LOI_META`).

Steel gives five phases like internal variables:

- $V1$  : proportion of the phase ferrite;
- $V2$  : proportion of the phase pearlite;
- $V3$  : proportion of the phase bainite;
- $V4$  : proportion of the phase martensite;
- $V5$  : proportion of the phase austenite.

The sum of all the phases must be equal to 1.0. If it is not the case (with a margin of 1 %), an alarm is emitted.

The data materials necessary must be indicated in `DEFI_MATERIAU` under the keyword `META_ACIER`.

```
/ 'ZIRC'
```

Is used to specify the execution of calculation for the metallurgical transformation (with cooling) of alloys of zirconium, a compact hexagonal phase to a cubic phase centered around  $800^{\circ}\text{C}$  (the selection of this model is done according to the keyword `LOI_META`).

Zircaloy gives three phases like internal variables:

- $V1$  : proportion of the cold phase  $\alpha$  ;
- $V2$  : initially without significance and obligatorily no one; for a postprocessing, fraction of phase  $\alpha$  is data by  $V1+V2$  ;
- $V3$  : proportion of the hot phase  $\beta$  .

The sum of all the phases must be equal to 1.0. If it is not the case (with a margin of 1 %), an alarm is emitted.

The data materials necessary must be indicated in `DEFI_MATERIAU` under the keyword `META_ZIRC`.

## 3.4.2 Operand `LOI_META`

```
If RELATION = 'STEEL'  
{  
    ◇ / LOI_META = 'WAECKEL', [DEFECT]  
}  
If RELATION = 'ZIRC'  
{  
    ◇ / LOI_META = 'EDGAR', [DEFECT]  
}
```

Is used to specify the metallurgical model used:

- For steel, the model of Waeckel (see R4.04.01);
- For Zircaloy, model EDGAR (see R4.04.04).

The model of Waeckel adds three internal variables to those describing the phases of steel:

- $V6$  : austenitic size of grain;
- $V7$  : temperature at the points of Gauss;
- $V8$  : martensitic temperature of transformation.

Model EDGAR adds two internal variables to those describing the phases of Zircaloy:

- $V4$  : temperature with the nodes;
- $V5$  : time corresponding is at the initial temperature of transformation to balance if the fraction of phase  $\alpha_1$  is worth initially, that is to say at the temperature of end of transformation to balance if the fraction of phase  $\alpha_0$  are worth initially. This variable is used to calculate speed with the heating, respectively with cooling (method of the slipping secant), which is used to determine the initial temperatures of transformation to the heating or cooling.

## 3.4.3 Operands `ALL / GROUP_MA`

```
◇ / ALL = 'YES',  
/ GROUP_MA = lgrma,
```

The meshes specify on which the model is used and allows DEto affect calculation that on under part of the total grid.

## 3.5 Keyword `ETAT_INIT`

```
◆ ETAT_INIT =  
  
◆ / META_INIT_ELNO = phasinit,
```

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```
/ EVOL_THER = temper
```

Initial metallurgical state.

Caution: The thermal structure of data `EVOL_THER` for the initial state must be the same one as that enriched by the order.

### 3.5.1 Operand `META_INIT_ELNO`

```
/ META_INIT_ELNO = phasinit
```

Defines the assignment of the field of internal variables initial constant by element starting from a map defined by `CREA_CHAMP`. Only the variables whose initial assignment has a direction are to be informed. One thus informs only the variables corresponding to a proportion of phase, more possibly that corresponding in keeping with austenitic grain if it is not worthless.

In the case of 'ACIER', one informs obligatorily all phases and size of grain, if not the code stops in fatal error.

If the user did not inform the sum of the cold phases correctly, it is the code which will replace by the sum calculated starting from the data. An alarm will then be emitted.

In case of 'ZIRC', one informs obligatorily all phases and time corresponding to the initial temperature of transformation to balance if not the code stops in fatal error.

### 3.5.2 Operands `EVOL_THER / NUME_INIT / INST_INIT / PRECISION / CRITERION`

```
/ EVOL_THER = temper
  ◆ /NUME_INIT = nuini_temper,
    / INST_INIT = to,
  ◇ /CRITERE = 'RELATIVE'
    ◇ PRECISION = /1.E-6
      / prec
    /CRITERE = ' ABSOLU'
    ◆ PRECISION = /prec
  ),
```

The concept defines `evol_ther` in which one will extract the initial state from which calculation will be carried out. This concept must contain metallurgical sizes.

The definition of the initial state can be done by stored sequence number or moment associated with calculation.

`NUME_INIT` the definition starting from the stored sequence number allows and `INST_INIT` the definition as from the moment of calculation allows.

In this case, `PRECISION` and `CRITERION` allow to define the precision and the criterion according to which the extraction will be carried out. If it `CRITERION = 'ABSOLUTE'` is selected, it is obligatory to inform the field `PRECISION`; for `CRITERION = 'RELATIVE'`, a precision of  $1.E-6$  by default is given, and can be possibly modified by informing the field `PRECISION`.

### 3.6 Operand `OPTION`

```
◇ OPTION =
```

```
| 'DURT_ELNO'
```

Hardness with the nodes by element starting from the metallurgical phases (cf [R4.04.01]).

```
| 'DURT_NOEU'
```

Hardness with the nodes starting from the metallurgical phases (cf [R4.04.01]).

```
| 'META_ELNO'  
Metallurgical proportion of phase to the nodes by elements.  
  
| 'META_NOEU'  
Metallurgical proportion of phase to the nodes.
```

## 4 Example in the case of a steel

```
# CREATION OF THE FIELD OF INTERNAL VARIABLES INITIAL (FERRITE 70%, BAINITE  
30% and the rest with zero)  
  
phasinit = CREA_CHAMP (OPERATION = 'AFFE',  
                      TYPE_CHAM = 'CART_VAR2_R',  
                      GRID = e-mail,  
                      AFFE = _F ( ALL = 'YES',  
                                NOM_CMP = ('V1', 'V2', 'V3', 'V4', 'V5', 'V6',  
                                'V7'),  
                                VALE = (0.7, 0.0, 0.3, 0.0, 0.1, 0.0)),  
  
# CALCULATION OF THE THERMAL EVOLUTION  
  
temple = THER_LINEAIRE ( MODEL = moth,  
                       CHAM_MATER = chmat,  
                       EXCIT = _F (LOAD = chth1),  
                       INCREMENT = (LIST_INST= lr8),  
                       TEMP_INIT = (VALE = 700),)  
  
# CALCULATION OF THE EVOLUTION OF THE METALLURGICAL PHASES  
  
temple = CALC_META ( reuse = temple,  
                   MODEL = moth,  
                   CHAM_MATER = chmat,  
                   RESULT = temple,  
                   ETAT_INIT = _F (META_INIT_ELNO = phasinit),  
                   BEHAVIOR = (RELATION = 'ACIER',  
                   ALL = 'YES'))
```