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The toughness module of the PERFECT platform: A predictive tool for the fracture toughness of RPV steels

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A B S T R A C T

The PERFECT project of the 6th Framework Program aims at developing a predictive tool for irradiation effects on Reactor Pressure Vessel steels. In this work, we focuse on the mechanical part of the numerical platform, the Toughness Module. Its main objective is to predict the probability of failure of the considered RPV steel, using more or less complex approaches. Six submodules are integrated in the Toughness Module. Three of them allow to estimate the macroscopic stress–strain curve of the material and the three others allow to predict the toughness drop of the material due to irradiation.

1. Introduction

In the framework of the PERFECT project (Prediction of Irradiation Damage Effects in Reactor Components) of the 6th Framework Program, predictive tools for the mechanical behaviour of Reactor Pressure Vessel (RPV) materials have been developed and integrated in a dedicated software. Different methodologies can be used and compared to predict the effect of irradiation on material properties.

Recent advances in fracture mechanics provide to use multi-scale modelling approaches to predict the fracture toughness. To compute the macroscopic stress–strain response of RPV steels, several methodologies are at present classically used to obtain the effective plastic behaviour from microstructural informations. At the micro-scale, computations are classically performed on representative microstructure using F.E. techniques. At the Representative Volume Element (RVE) scale, homogenisation methods are widely developed. Starting with such crystal plasticity based results, micromechanical methods to predict the fracture toughness have been investigated and successfully applied. The purpose of the paper is to present the available multi-scale modelling methodologies which have been integrated in the Toughness Module and which can represent the state of the art for the prediction of irradiation effect on mechanical behaviour of bainitic steels.

The two main objectives of the Toughness Module are to predict the stress–strain curve and to estimate the fracture behaviour of RPV steels as function of irradiation level. To reach this goal, several paths of analysis at three different scales have been integrated in the numerical platform. The various methods, at the micro scale, at the RVE scale and at the specimen scale can be linked up together. The scheme of the linkage is presented in Fig. 1. Some models use simple correlations as the Correlation sub-module based on the Master Curve shift. Other approaches are more complex as the SubModelling sub-module which proposes crystal plasticity based computations in order to predict the probability of brittle fracture for a RVE.

The Toughness Module is an end-product that integrates SPIII (RPV Mechanics) models. It uses output from RPV2, that is the microstructural hardening due to irradiation, in order to estimate the corresponding toughness drop. In a first part, we present the general structure of the Toughness Module. In a second part, a description of the different sub-modules, their integration in the structure of the numerical tool and their chaining is given. Each sub-module will then be presented in detail as it is integrated in the platform at present.

2. Description of the Toughness Module

The Toughness Module integrated in the PERFECT platform presented in Bugat et al. [4] provides the prediction of the fracture behaviour of the irradiated RPV steel. The irradiation effects on material properties can be estimated using various approaches at different scales.

The Toughness Module is divided in two main modules, the FlowBehaviour module and the FractureBehaviour module, which can be chained (see Fig. 1). The FlowBehaviour module provides the macroscopic behaviour of the RPV steel. Three different models are available to reach this goal. The FractureBehaviour module allows to estimate the decrease of toughness of RPV steel due to

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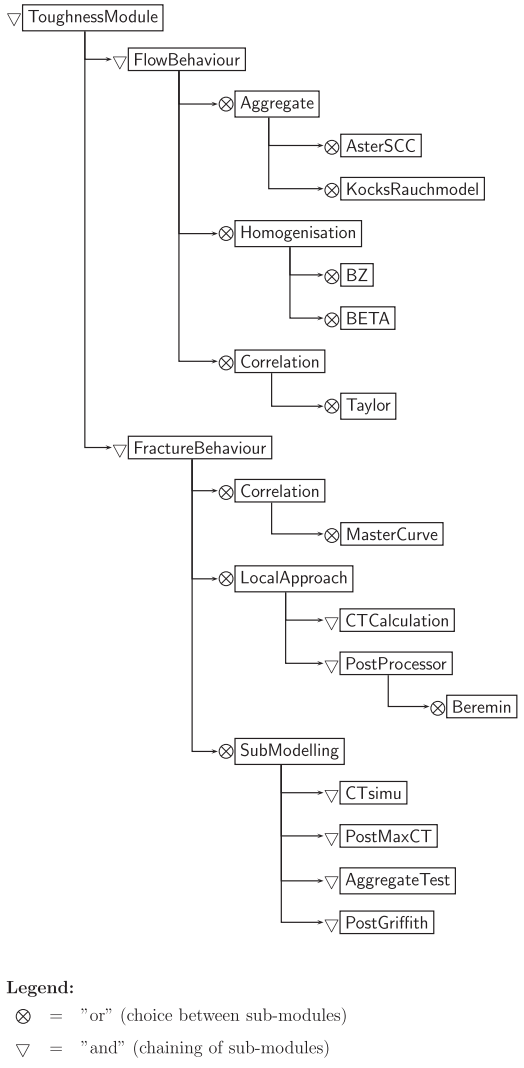

Fig. 1. The Toughness Module tree-view: the Toughness Module is divided into two sub-modules, the FlowBehaviour sub-module and the FractureBehaviour sub-module. Each sub-modules contains different approaches which provide the same results. This tree-view shows which sub-modules can be chained or not.

irradiation. A choice between three different models more or less complex is also proposed.

The FlowBehaviour module allows to estimate the macroscopic behaviour of the irradiated or unirradiated RPV steel, starting from information from the output of RPV-2 module, that is the microscopic behaviour at the bainitic lath level. Three different approaches are proposed to determine the macroscopic stress–strain curve of the steel which are the following:

- the Aggregate sub-module which allows to provide the macroscopic tensile curve using a Finite Element (F.E.) simulation of a representative volume element (RVE) of $18 * 18 * 18$ elements containing 100 grains, computed with a Cailletaud–Meric [12] type single crystal law and *Code_Aster*[1] as F.E. code.
- the Homogenisation sub-module which provides the macroscopic stress–strain curve using a tensile simulation on a RVE containing 100 grains. In this method, the tensile test is performed on one element mesh representating a 100 grains RVE with a homogenisation model which accounts for the interaction between grains.
- the Correlation sub-module which allows to predict the increase of yield stress due to irradiation using the Taylor correlation. It supposes that the increase of yield stress is proportional to the increase of the critical resolved shear stress (CRSS).

The FractureBehaviour module allows to estimate the fracture toughness drop of RPV steels due to irradiation effects from informations on the irradiated macroscopic behaviour. Three different approaches are proposed:

- The Correlation sub-module which is based on the Master Curve model (Norm-ASTM [7]). It provides the failure curve of a 1T–CT at a given temperature according to the Master Curve model.
- The LocalApproach sub-module provides the failure curve of a 1T-CT at a given temperature, according to the Beremin local approach model [2]. A F.E. simulation of a 1T-CT specimen is performed with the local behaviour defined by the tensile curve of the irradiated material.
- The SubModelling sub-module which provides the local probability of fracture from metalurgical informations as carbides size distribution and knowing of the mechanical fields. Applying the Griffith criterion to the carbides, a statistical analysis allows to determine the probability of fracture and its temperature dependency.

3. Structure of the end-products and their chaining

The Toughness Module proposes several paths of analysis, from the most simple which uses simple correlations for mechanical behaviour prediction of irradiated material, to the most complex but also the most accurate, which uses recent advances in multiscale modelling. The tool is divided in two main parts: the first part's objective is to predict the macroscopic behaviour of the irradiated material and the second part goal is to estimate the fracture toughness drop due to irradiation. The second part uses the output from the first. For example, the tensile curve extracted from the Homogenisation sub-module is an input of the LocalApproach sub-module. The general structure and the possible linkage between the various models are shown Fig. 2.

4. Macroscopic behaviour prediction of RPV steel

Three different models are proposed to estimate the macroscopic behaviour of the material. They are presented in detail in the following.

4.1. *Aggregate* module

The first model proposed is a tensile test on a aggregate with $18 * 18 * 18$ elements containing 300 grains. The aggregate is supposed to be representative of the microstructure. Each Gauss point belonging to an element of a given grain follows a single-crystal plasticity law which could be of Cailletaud type single crystal law or the Kocks-Rauch law. These two single crystal models are described in the following.

4.1.1. *AsterSCC sub-module*

The AsterSCC sub-module allows to estimate the macroscopic stress–strain curve using a F.E. tensile test on a polycrystalline aggregate and a single crystal behaviour law of type Cailletaud-Meric. Two slip system families are considered $\{111\}-\langle 110\rangle$ and $\{111\}-\langle 112\rangle$. The main equations are reminded in Fig. 3.

[1] http://www.code-aster.org.

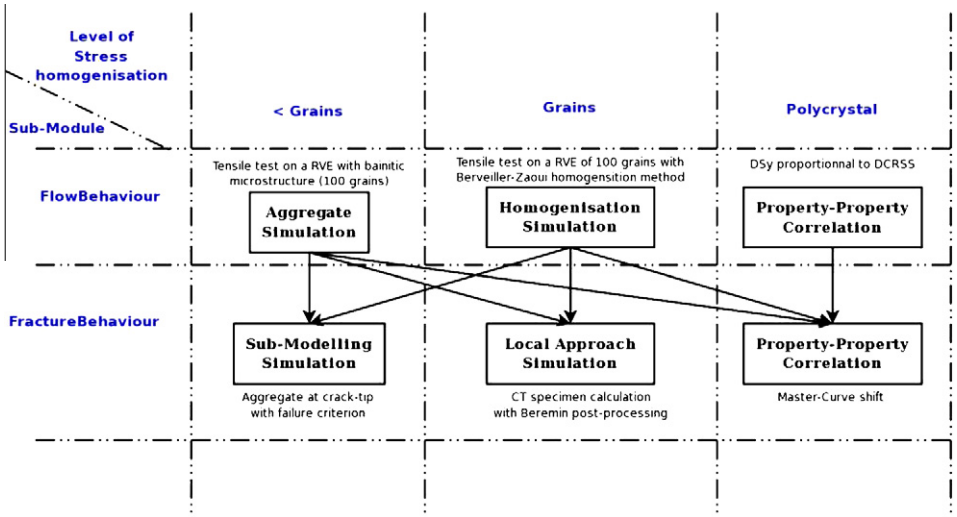

Fig. 2. The Toughness Module is divided into two main sections corresponding to the two rows of the Toughness Module matrix: the flow behaviour section and the fracture behaviour section. Each section is itself divided into three different levels which correspond to the columns of the Toughness Module matrix: the microscopic scale, the RVE scale and the specimen scale. The possible chaining between the various sub-modules is represented by the arrows.

This formulation has been originally presented in Méric et al. [12]. The classical decomposition of strain rate into elastic (ε^e) and plastic part ($\underset{\sim}{\varepsilon^p}$) is adopted (Eq. (1)). Plastic strain rate is calculated from the sum of the elementary slip on the crystalline slip systems in Eq. (4). The crystallographic particularities are defined by means of the orientation tensor $\mathbf{P}^s$ in relation 4. Slip systems are geometrically defined by vectors $\underline{\mathbf{n}}^s$ and $\underline{\mathbf{l}}^s$ which are respectively the normal to the slip plane and the slip direction. Each slip rate $\dot{\gamma}^s$ depends on the resolved shear stress τ^s, following the Schmid law. A phenomenological Norton-like viscoplastic flow rule is adopted (Eq. (5)). The effect of the self and latent hardening are introduced by the means of the interaction matrix h_{sr}.

The tensile test is performed on an aggregate F.E. mesh. The construction of the aggregate is based on the Voronoi polyhedra model [8]. This approach is widely used in material science to represent real-like polycrystals [1,10]. The method is based on the space division by Voronoi polyhedra. They were formally defined as "zones of influence" of a particular set of points [6]. The polyhedra centers can distributed in space, following a random law. A repulsion distance is introduced to control a minimum size of the grains and to obtain a regular grain size distribution. Each grain is identified in the mesh as a set of hexahedric elements and oriented following the orientations given in the texture file.

A tensile test is performed on the aggregate F.E. mesh using F.E. code *Code_Aster*. The boundary conditions applied on the aggregate are the following:

- $U_z = 0$ for nodes which belong to the plane $z = 0$;
- $U_z = \varepsilon \times$ time for nodes which belongs to the plane $z = 1$. ε is the imposed deformation, knowing that the size of the aggregate is 1;

$$\underset{\sim}{\dot{\varepsilon}} = \underset{\sim}{\dot{\varepsilon}}^e + \underset{\sim}{\dot{\varepsilon}}^p \quad (1)$$

$$\tau^s = \underset{\sim}{\sigma}^g : \underset{\sim}{\mathbf{P}}^s = \frac{1}{2}\,\underset{\sim}{\sigma}^g : (\underline{\mathbf{n}}^s \otimes \underline{\mathbf{l}}^s + \underline{\mathbf{l}}^s \otimes \underline{\mathbf{n}}^s) \quad (2)$$

$$x^s = c\alpha^s \;;\; r^s = r_0 + bQ\sum_r h_{sr} q^r = r_0 + Q\sum_r h_{sr}\left\{1 - e^{-bv^r}\right\} \quad (3)$$

$$\dot{\gamma}^s = \dot{v}^s \mathrm{sign}(\tau^s - x^s) \;;\; \underset{\sim}{\dot{\varepsilon}}^p = \sum_s \underset{\sim}{\mathbf{P}}^s \dot{\gamma}^s \quad (4)$$

$$\dot{v}^s = \left\langle \frac{|\tau^s - x^s| - r^s}{K} \right\rangle^n \text{ with } \langle x \rangle = \max(x, 0) \text{ and } \dot{v}^s(t=0) = 0 \quad (5)$$

$$\dot{\alpha}^s = \dot{\gamma}^s - d\alpha^s \dot{v}^s \text{ with } \alpha^s(t=0) = 0 \;;\; \dot{q}^s = (1 - bq^s)\dot{v}^s \quad (6)$$

Fig. 3. Cailletaud-Méric single crystal plasticity model.

- $U_y = 0$ for nodes which belongs to the plane $y = 0$;
- $U_x = 0$ for nodes which belongs to the plane $x = 0$;

4.1.2. Kocks-Rauch sub-module

In this sub-module, a modified Kocks-Rauch formulation for single crystal plasticity developed in Libert et al. [11] is proposed in order to estimate the macroscopic stress–strain curve from a tensile test on a tri-dimensional Voronoi type mesh. It allows to describe both thermal and athermal regime with a dislocation density based crystal plasticity model. The main equations of the model are recalled in Fig. 4. The applied shear stress on a slip system is divided into three parts (see Eq. (7)):

- τ_0 is the critical resolved shear stress. The irradiation effect is supposed to affect only this parameter
- the thermal component corresponds to the stress needed to overcome short range obstacles
- τ_μ, the athermal stress component which allows to overcome long range obstacles

The plastic flow law is introduced in Eq. (8) where the activation enthalpy is given by a phenomenological law (Eq. (9)) proposed by Kocks et al. [9]. The hardening law is formulated following Teodosiu law: the critical shear stress on each slip system is proportional to the square root of dislocation densities on all slip system and integrates Rauch description [13] for the effect of the thermally activated double kink mechanism on the

$$\tau = \tau_0 + \tau_\mu + \tau_{\text{eff}} \quad (7)$$

$$\dot{\gamma}^s = \dot{\gamma}^0 exp\left(-\frac{\Delta G(\tau^s_{\text{eff}})}{kT}\right) \quad (8)$$

$$\Delta G(\tau^s_{\text{eff}}) = \Delta G_0 \left(1 - \left(\frac{\tau^s_{\text{eff}}}{\tau_R}\right)^p\right)^q \quad (9)$$

$$\tau^s_\mu = \frac{(\mu b)^2 \sum_u a^{su}\rho^u}{|\tau^s - \tau^0|} \; with \; |\tau^s| > \tau^0 \; and \; \tau^s_{\text{eff}} > 0 \quad (10)$$

$$\dot{\rho}^s = \frac{\dot{\gamma}^s}{b}\left(\frac{1}{d} + \frac{\sqrt{\sum_{u\neq s}\rho^u}}{K} - g_c\rho^s\right) \quad (11)$$

Fig. 4. Kocks–Rauch behaviour model.

curvature of dislocations pinned by forest obstacles (Eq. (10)). The dislocation densities evolution law is given in Eq. (11).

4.2. Homogenisation module

The Homogenisation module allows to estimate the macroscopic behaviour of the material from a tensile simulation on a RVE which contains 100 grains. A set of constitutive equations are needed to account for both:

- the behaviour of a single grain (defined as a single crystal)
- an "interaction law" (or homogenisation model) that will correlate the behaviour of the individual grains to the macroscopic behaviour of the aggregate (defined as the polycrystal).

In the Homogenisation module, different models can be used. They differ in the use of a specific single cystal behaviour law and on the chosen homogenisation scheme. All homogenisation models used in the module are based on a self-consistent approach. Each grain of the polycrystal is supposed to be embedded in the so-called "equivalent medium" which behaviour is the macroscopic behaviour of the aggregate.

4.2.1. The BZ sub-module

This sub-module integrates the Berveiller-Zaoui homogenisation model and single crystal behaviour law which is the Cailletaud type approach with one non-linear isotropic hardening and one kinematic isotropic hardening. The Berveiller-Zaoui homogenisation model [3] is often used to identify the single crystal behaviour parameters from a tensile test. It does not require specific parameters. The main characteristic of the approach relies on the formulation which relates the local mechanical fields to the macroscopic mechanical fields. Indeed, the local average stress in the grain i is related to the macroscopic stress thanks to the following relation:

$$\underset{\sim}{\sigma}^i = \underset{\sim}{\Sigma} + \frac{\mu}{1+\frac{3}{2}\mu\frac{E_{eq}}{\Sigma_{eq}}}\left(\underset{\sim p}{\mathbf{E}} - \underset{\sim p}{\varepsilon}^i\right) \tag{12}$$

The capital letters denote for the macroscopic mechanical fields, and the small letters denote for the local mechanical fields. μ is the shear modulus. $\underset{\sim p}{E}$ is the plastic strain tensor and $\underset{\sim p}{\varepsilon}^i$ is the plastic strain tensor of a grain. Σ_{eq} is the equivalent macroscopic stress and E_{eq} is the equivalent macroscopic strain. To obtain the macroscopic plastic deformation of the RVE, one has to sum the contribution of all grains i. Macroscopic plastic strain is linked to macroscopic stress by Hook's law.

4.2.2. The Beta sub-module

In this sub-module, the Beta homogenisation approach [5] is used coupled with a single crystal behaviour law of type Cailletaud model. In the Beta model, the accommodation term for a given phase introduces the difference between the macroscopic plastic strain and the plastic strain of the considered phase, including an accommodation factor which decreases with plastic deformation, that reduces stress heterogeneities. For each phase, we can define one "internal stress" which depends non-linearly on the plastic deformation at the present time, using the term β. The concentration rule becomes:

$$\underset{\sim}{\sigma}^i = \underset{\sim}{\Sigma} + \mu(\underset{\sim}{\mathbf{B}} - \underset{\sim}{\beta}^i) \quad \text{with } \underset{\sim}{\mathbf{B}} = \langle\underset{\sim}{\beta}\rangle = \sum_i f^i\beta^i \tag{13}$$

If we consider a polycrystalline aggregate, the slip systems rate is introduced in the following relation:

$$\dot{\underset{\sim}{\beta}}^i = \dot{\underset{\sim p}{\varepsilon}}^i - D\left(\underset{\sim}{\beta}^i - \delta\,\underset{\sim p}{\varepsilon}^i\right)\|\dot{\underset{\sim p}{\varepsilon}}^i\| \tag{14}$$

4.3. Correlation module

The correlation sub-module uses a simple correlation model, the Taylor correlation approach in which it is assumed that the increase of yield stress $\Delta\sigma_Y$ of the polycrystal is proportionnal to the increase of critical resolved shear stress τ_c of its composing single crystals (the grains). The main relation of the model are the following:

$$\sigma_Y^{irr} = \sigma_Y^0 + \Delta\sigma_Y \tag{15}$$

$$\Delta\sigma_Y = \alpha\tau_c \tag{16}$$

The Taylor factor α usually lies between 2 and 3. τ_c is the CRSS, σ_Y is the yield stress and 0 as superscript stands for the initial state and irr for the irradiated state.

5. Toughness estimation of RPV steel

The FractureBehaviour module allows to estimate the fracture toughness of the material due to the increase of hardening of the irradiated RPV steel, knowing the irradiated macroscopic behaviour evaluated thanks to the FlowBehaviour module.

5.1. Correlation module

This sub-module is based on an analytical fracture model, the Master Curve model. The Correlation module consists of:

- a parameter that allows to estimate the shift of reference temperature T_0 from the shift of yield stress;
- a classical Master Curve formulation, using the corresponding shifted T_0.

The Master Curve describes the failure probability of the ferritic steel P_r with respect to the material loading K,according to:

$$P_r = 1 - exp\left\{-\left[0.9124\left(\frac{K-K_{min}}{K_{med}-K_{min}}\right)\right]^4\right\} \tag{17}$$

K_{min} is the minimum K value to reach failure and K_{med} is defined by:

$$K_{med} = 30 + 70\times\exp[\gamma(T-T_0)] \tag{18}$$

with T_0 the reference temperature of the steel, T the test temperature and γ the shape factor equal to 0.019.

The needed parameters for the module are:

- the initial yield stress σ_{Y0} of the material;
- the irradiated yield stress σ_Y;
- the initial Master Curve model for the unirradiated material, characterised by an unirradiated temperature T_0, the shift parameter and the testing temperature for the failure curve.

5.2. LocalApproach module

In this sub-module the prediction of toughness is based on local approach to fracture models. A F.E. simulation is performed on a 1T–CT specimen with the tensile behaviour of the irradiated material. It is chained with a post-processing that uses a local approach model in order to estimate the fracture toughness.

5.2.1. CTCalculation sub-module

This sub-module is a F.E. simulation on a 1T–CT specimen in 2D-plain strain. The classical von Mises elasto-plastic behaviour of the irradiated material is given by the tensile curve which is

an output of the FlowBehaviour module. The element size at crack tip is 50 μm. The CTCalculation module produces a file which contains the stress and strain fields and the loading curve. This module is usually followed by a local post-processor.

5.2.2. Post-processor sub-module

The post-processing module integrated in the LocalApproach module allows to predict the fracture toughness probability using the classical post-processor of type Beremin. The Beremin model relies on the weakest link theory and estimates the cumulated failure probability of a given structure as a function of an elementary failure probability on a reference volume V_0. This elementary probability is correlated to the probability to find a critical size defect in the volume V_0. If we consider a Weibull statistics with two parameters, the cumulated failure probability is written:

$$P_f(\sigma_w) = 1 - \exp\left[-\left(\frac{\sigma_w}{\sigma_u}\right)^m\right] \tag{19}$$

m describes the dispersion around the mean value and σ_u controls the mean value. The Weibull stress σ_w is defined over the whole structure as the weighted sum of the maximum principal stress over the plastified volume. The model relies on the hypothesis of a nucleation of micro-defects controlled by plastic deformation. σ_w can then be defined as follows:

$$\sigma_w = \sqrt[m]{\sum_i \left(\sigma_I^i\right)^m \exp\left(-\frac{m\varepsilon_I}{k}\right)\frac{V_i}{V_0}} \tag{20}$$

V_0 is the reference volume on which the mechanical fields are averaged in order to fulfill the hypothesis of homogeneous fields. σ_I^i refers to the maximum principal stress of the volume i. In the platform, three input parameters are required for the Beremin post-processing which are the elementary volume V_0, the dispersion coefficient m and the reference stress σ_u.

5.3. SubModelling module

The SubModelling module allows to evaluate the local probability of fracture from carbides sizes distribution and from computed local mechanical fields.

5.3.1. CTCalculation sub-module

In this sub-module, a 1T-CT calculation is performed. The 1T-CT simulation has strictly the same characteristics than in the LocalApproach module. Indeed, the computation is realised on a bi-dimensional specimen, in plane strain conditions with the tensile behaviour of the irradiated material, which is an output of the FlowBehaviour module. The element size at crack tip is 50 μm. The file resulting from the calculation contains all stress and strain fields which will then be post-processed in order to extract the maximum stress and strain at the crack tip.

5.3.2. PostMaxCT sub-module

The PostMaxCT post-processor allows to extract the maximum stress and strain at the crack tip of the CT specimen which is computed in the previous sub-module. The results of the PostMaxCT post-processor is an input of the Aggregate sub-module.

5.3.3. Aggregate sub-module

In this sub-module, a F.E. simulation on a tri-dimensional polycrystalline aggregate is realised using a single crystal behaviour law of type Cailletaud-Meric. An isotropic texture is proposed by default. Homogeneous strain boundary conditions are applied on the polycrystal. The applied loading on the polycrystalline aggregate is the deformation extracted from the crack tip on the CT specimen. The output data of the Aggregate sub-module are the local stress and strain fields at each Gauss point in the volume, and each time step.

5.3.4. PostGriffith sub-module

The last sub-module of the chain provides the cumulated fracture probability of the RVE from a deterministic cleavage criterium, applied to different realizations of default size and coupled with the weakest link hypothesis. The PostGriffith sub-module can be developed in several steps:

- the first step consists of the projection of the stress tensor on the cleavage planes (σ_{cleavage});
- the maximum equivalent stress on the cleavage planes is then extracted $\left(\sigma^{\max}_{\text{cleavage}}\right)$;
- the biggest carbides ($r_{\max}$) is detected in the RVE;
- the time t_i and the value of the corresponding stress is recorded if $\sigma_{\text{Griffith}} < \sigma^{\max}_{\text{cleavage}}$;
- the stress value is noted as the fracture stress σ_{rupture} for the time t_i which is the shorter one;
- the cumulated fracture probability is then determined. It corresponds to the average of the fracture stress σ_{rupture} over all the realizations.

6. Conclusions

Multi-scales modelling of macroscopic behaviour and fracture properties of RPV steels are proposed in the Toughness Module, developed in the framework of the PERFECT project, and integrated in the PERFECT numerical platform. The specifications of the Toughness Module have been built in common with SPIII "RPV Mechanics". Finite Element models and simple correlation models are proposed in the present version of the product. It uses the outputs from RPV2 that is the microstructural hardening due to irradiation and metallographic analysis results as informations on the microstructural morphology, the crystallographic texture and the carbide size distributions for instance. The Finite Element code used is *Code_Aster*. The Toughness Module sub-modules can be linked together following specific modelling strategy. It provides both macroscopic mechanical response, local stress and strain fields in ferritic steel and local probability of fracture using statistical laws. It is also of strong interest to investigate the effect of specific parameters as the temperature dependance on local stress fields for instance. Future works will focuse on the Toughness Module improvement with the development and integration of new models and approaches, including more informations on stress heterogeneities in order to obtain an accurate estimation of the fracture behaviour of RPV steels.

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