Micromechanical modelling of cohesive thermoelastic steady-state and transient cracking in polycrystalline materials

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Abstract

In this paper a micromechanical formulation is proposed for modelling thermoelastic intergranular and transgranular damage, and microcracking evolution in brittle polycrystalline materials. The model is based on a multi-region boundary element approach combined with the dual boundary element formulation. Polycrystalline microstructures are created through a Voronoi tessellation algorithm. Each crystal has an elastic isotropic behaviour and multi-phase aggregates have been considered. Damage evolution along (inter- or trans- granular) interfaces is modelled using thermo-mechanical cohesive laws and, upon failure, non-linear frictional contact analysis is introduced to model separation, stick or slip. Steady-state and transient thermoelastic formulations have been modelled and numerical simulations are presented, not only to demonstrate the validity but also to study the physical implications of the proposed formulation, in comparison with other numerical methods as well as experimental observations and literature results.

Keywords: thermo-elasticity, transgranular, intergranular, multi-phase polycrystalline, cohesive microfracture, boundary element method

1. Introduction

It is well established that failure and microcracking of polycrystalline materials depend on a number of factors \cite{1,2}: single grain’s elastic properties, material anisotropy, grain’s morphology, grain’s size distribution in the aggregate, boundary vs grain critical energies and mismatches between adjacent crystals are a few examples. However a pivotal role in the development of damage and the residual life of these materials is played by the effect of temperature. The thermal effect can be considered either because of long exposure of the

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component to high temperature or due to cooling down from fabrication to room temperature or for other thermal treatments such as quenching; temperature excursion has a great influence, but as it has been mentioned in [1], it is the material crystallographic structure that affects the initiation of micro-cracking: (i) non-cubic single-phase polycrystalline aggregates experience differential expansion due to thermal expansion anisotropy (TEA) in single phase materials; (ii) differential thermal expansion due to mismatch of thermal expansion/contraction, even in isotropic but multi-phase polycrystalline materials, or also due to transient temperature gradients might generate residual stresses between adjacent grains and damage onset could occur. This phenomenon is called thermal-expansion-induced microcracking.

In polycrystalline materials the modes of fracture are well recognised and can be categorized as follows: brittle intergranular and transgranular cracking, ductile failure and at high temperature creep has to be taken into account. It is worth noting however that Blendell and Coble in [3] have measured stresses development due to thermal expansion anisotropy in $Al_2O_3$ and showed that the microstructure does not experience any stress relaxation until very high temperature, close to the annealing. Thus in this work the effect of creep has not been considered since the thermal loading has been applied within the range of temperatures that guarantees no stress relaxation. Moreover still from the experimental findings in [3], the authors have extrapolated the stress-free temperature, from which it is possible to approximate analytically the maximum local stress due to differential thermal expansion. Results in the present work will be shown in good agreement with these literature results.

Experimental methods may be used for such investigations, even though sometimes they might be expensive and time consuming due to specific required techniques. Experimental results on grain size dependence and thermal expansion anisotropy were presented by Rice et al. in [4,5] as well as spontaneous cracking in [6]. Experiments and simulations were run by Yousef et al. [7] where residual stresses due to cooling from stress free status has been investigated. Thermal expansion anisotropy has been studied also in [8] where the effect of microcracking due to local thermal expansion mismatch has a substantial influence on the damage evolution in the polycrystalline aggregate.

A popular and powerful approach to investigate such mechanisms is the use of computational micromechanic models. Finite Element Method (FEM) has been widely used thanks to the availability of commercial software. Intergranular failure has been studied by modelling grains’ interfaces as cohesive surfaces. 2D models of polycrystals are the most common in literature, especially when fracture and damage propagation are investigated; these phenomena are the result of a synergism of mechanisms that two-dimensional analysis allow to capture accurately without the complexity introduced by fully 3D models. The most popular cohesive failure models have been proposed by Camacho and Ortiz, who studied impact damage and propagation of multiple cracks in 2D [9], and the potential based laws by Tvergaard [10] and Xu and Needleman [11]. An extensive review of cohesive traction-separation laws for fracture
has been done by Park and Paulino [12]. Competition between inter- and trans-granular
damage has been investigated by many authors, and examples are: Sukumar et al. [13], Qian
and Li [14] and Lin et al. [15]. Espinosa and Zavattieri [16, 17] have studied the dynamic
fragmentation of ceramics using a cohesive finite element formulation and the role of residual
stresses as well as thermal induced microcracking have been investigated.

However when studying thermo-elastic problems, interfaces or cracks may act as barriers
for the heat propagation [18], so in the framework of cohesive damage evolution, thermo-
mechanical cohesive relationships have been developed. William et al. [19] examined the
degradation of interfaces in heterogeneous materials due to thermal and mechanical damage;
other examples of thermo-mechanical cohesive zone models are the works by Sapora and Paggi
[20], Wu and Wriggers [21] and Özdemir et al. [22], where finite element models have been
developed in order to describe coupled thermoelastic debonding, temperature and humidity
jump across a cohesive crack and the concept of thermal damage has been introduced.

Image analysis has been proposed in [23] to process real solar cell pictures, identify grains
and grain boundaries in polycrystalline silicon, and generate finite element meshes. More
recently a phase-field approach has been combined to the cohesive model to study intergranular
and transgranular fracture in solar-grade Silicon with a FE-based technique [24].

Although FEM is widely utilised, in recent years Boundary Element Method (BEM) has also
gained much popularity [25]. Application of boundary element formulation to intergranular
fracture processes in polycrystalline materials is due to Sfatos and Aliabadi [26]. Benedetti
and Aliabadi [2] have presented a three-dimensional grain-boundary micromechanical model
for intergranular fracture. More recently Benedetti et al. [27] investigated the integrantular
stress corrosion cracking. Dual Boundary Element Method (DBEM) formulation to deal with
coplanar surfaces (cracks) embedded within the same domain is due to Portela, Aliabadi and
Rooke [28, 29]. The extension of DBEM to thermoelastic problems is due to Prasad and
recently Geraci and Aliabadi [1] have presented a cohesive formulation for intergranular and
transgranular damage propagation, with particular attention to the factors influencing their
interaction and hence the mode of fracture; the extension to the steady-state thermoelastic
damage model for orthotropic polycrystals has been presented instead in [32].

In this paper a cohesive thermoelastic formulation with boundary element method is
presented for two-dimensional modelling intergranular and transgranular damage propagation
in polycrystalline aggregates, under the effect of thermo-mechanical loading, for the first time.
Since the development of the BE formulation for the transition between inter- and trans-
granular damage has been already presented in [1], the current work deals with the extension
of that model to the thermoelastic analysis. It is worth noting that not only steady-state
but also transient formulation will be shown, since thermal shocks are very common in such
materials. Effects of thermal shocks on cracks propagation have been investigated in [33] and
The possibility to model multi-phase polycrystalline material is also considered in order to investigate the role of differential thermal expansion on either residual stresses and damage nucleation between adjacent grains. Multi-phase micromechanical damage models have been extensively studied in literature, i.e. metals, titanium alloys [35] or ceramic composites; among the latter particular attention has been paid to Al$_2$O$_3$ with dispersed particles of ZrO$_2$, TiN/TiC/TiO$_2$, BN and SiC [36]. Mechanical properties and fracture behaviour have been investigated and it has been shown that for example ceramic composite made of silicon carbide and alumina (Al$_2$O$_3$/SiC) can have enhanced properties compared to the respective pure materials [36, 37]. However it has also been highlighted that the addition of those particles have effects generally on two opposite behaviours, that make the improvement of mechanical and fracture properties dependent on the amount of particle dispersed in the main material: the presence of particles has a beneficial effect on toughness and strength, but at the same time it refines the grains during the sintering process; if the grains then are refined significantly the overall toughness at high percentages of SiC could decrease or be not as enhanced as in the case with smaller percentages of SiC particles. In this work such effect on grain refinement has not been studied because it is beyond the scope of the present analysis, hence only the strengthening effect of the additional phase is present.

Each grain is modelled as a single crystal with general isotropic mechanical behaviour and generic material orientation. The assumption of isotropy for polycrystalline materials can be explained by virtue of different reasons: 1) the materials considered have general 3D transverse isotropic behaviour, hence one crystallographic plane is isotropic; 2) the level of anisotropy for the remaining crystallographic planes is low; 3) the aim of the numerical tests presented in this paper is to show that not only does thermal-expansion-induced microcracking affect anisotropic microstructures, but it also influences isotropic aggregates if more than one phase is present, or even single-phase isotropic microstructures if these are subjected to thermal shocks.

Grain boundary interfaces as well as cracks within the grains are modelled using cohesive law which allows for nucleation and propagation of cracks under mixed mode conditions. As the generic interface/crack completely deteriorates within its cohesive regime, a non-linear frictional contact analysis is used in order to simulate sliding or sticking contact of free surfaces. The concept of a cohesive model has been extended to the heat conduction across the generic interface, where the heat flux has been considered dependent on the level of damage of the interface. In this way the presence of damage or fracture acts as a barrier for the heat conduction. Furthermore the effect of temperature on the elastic properties has been neglected in the present formulation.
2. Thermo-mechanical cohesive model

In [1] the details of the traction-separation laws used in this model have been presented extensively, thus here only the main conclusions will be summarized. When the opening of a cohesive interface is considered until complete de-cohesion along a generic angle $\phi$ the work of decohesion can be split into normal and tangential contribution. As the ratio between these two is evaluated, $G_{II}/G_I$ is obtained; when a potential cohesive law is used, this parameter is assumed implicitly equal to one, meaning that the damage propagation is path-independent. In the present work however, this hypothesis has been released so that the cohesive parameters are related through the following relationship:

$$\alpha = \beta^2 \frac{\delta u_n^{\text{crit}}}{\delta u_t^{\text{crit}}} \frac{G_{II}}{G_I}$$  \hspace{1cm} (1)

where the ratio $G_{II}/G_I$ can now be assigned arbitrarily. $\delta u_t^{\text{crit}}$ and $\delta u_n^{\text{crit}}$ are respectively the critical tangential and normal opening displacement of the generic cohesive interface. The traction-separation laws take the form:

$$\begin{cases} t_n &= T_{\text{max}} \left( 1 - \frac{d}{d} \frac{\delta u_n}{\delta u_n^{\text{crit}}} \right) \\ t_t &= \alpha T_{\text{max}} \left( 1 - \frac{d}{d} \frac{\delta u_t}{\delta u_t^{\text{crit}}} \right) \end{cases}$$  \hspace{1cm} (2)

where $d$ represents the damage status (monotonically increasing) of a cohesive surface, being $d = 0$ for pristine surfaces and $d = 1$ for completely failed ones.

$$d = \sqrt{\left( \frac{\delta u_n}{\delta u_n^{\text{crit}}} \right)^2 + \beta^2 \left( \frac{\delta u_t}{\delta u_t^{\text{crit}}} \right)^2}$$  \hspace{1cm} (3)

$\delta u_n$ and $\delta u_t$ are respectively the current normal and tangential displacement jumps of the interface.

In order to include the temperature field into this model, a similar approach has been used following [2], where the concept of thermal damage has been expressed as a “reduction in the effective conductivity”. Thus here the thermal cohesive law, which relates the temperature gradient to the flux, is expressed as:

$$q(d) = -k^e f(d) \frac{\partial \theta}{\partial n}$$  \hspace{1cm} (4)
Figure 1: Grains’ reference systems and modelling of interface

where \( k_{eff}(d) = (1 - d)k^l \) is an effective conductivity, \( \partial \theta / \partial n \) is the temperature gradient in the direction perpendicular to the interface and according to Fourier’s law the flux \( q \) is opposite to the gradient. \( k^l \) is the interface conductivity which can be calculated using the analogy between thermal and electrical resistance concepts. The heat flux through a plane wall can be expressed as:

\[
q = \frac{\Delta \theta}{R_{tot}} \tag{5}
\]

where \( \Delta \theta \) is the temperature difference and \( R_{tot} \) the total thermal resistance resulting from a series of \( N \) different layers with thicknesses \( L_i \) and conductivities \( k_i \):

\[
R_{tot} = \sum_{i=1}^{N} \frac{L_i}{k_i} \tag{6}
\]

By applying the above concept to the interface between two grains \( A \) and \( B \) (or to a transgranular interface) where the opening displacement between the two surfaces of the interface is \( \delta u_n \), it is plausible to consider the interface itself as a “multilayer wall” where each portion has thickness \( \delta u_n/2 \) (Figure 1) and conductivity depends on the conductivities of the materials of each grain. Using Eq. (6) one gets:

\[
R_{tot} = \frac{\delta u_n/2}{k_A} + \frac{\delta u_n/2}{k_B} = \frac{k_A + k_B}{k_A k_B} \frac{\delta u_n}{2} = \frac{\delta u_n}{k^l} \tag{7}
\]
The thermal cohesive law in Eq. (4) can be rewritten as:

\[ q(d) = -(1 - d) \frac{2k_A k_B}{k_A + k_B} \frac{\Delta \theta}{\delta u_n} \]  

(8)

Equation (8) is referred to the direction normal to the interface, but in the most generic case the conductivity \( k \) should be considered as a second order tensor:

\[
\begin{bmatrix}
q_t \\
q_n
\end{bmatrix} = -\begin{bmatrix}
k_{tt} & k_{tn} \\
k_{tn} & k_{nn}
\end{bmatrix} \begin{bmatrix}
\frac{\partial \theta}{\partial t} \\
\frac{\partial \theta}{\partial n}
\end{bmatrix}
\]  

(9)

where \( t \) is the tangential direction and \( n \) the normal direction to the interface. Moreover, the conductivity coefficients \( k_{ij} \) are related through thermodynamics principles and Onsager’s reciprocity [38, 39]:

\[ k_{11} > 0; \; k_{22} > 0; \; k_{11}k_{22} - k_{12}^2 > 0; \; k_{12} = k_{21} \]  

(10)

For general orthotropy, the conductivity matrix can be written as:

\[
k^{t-n} = \begin{bmatrix}
k_{tt} & k_{tn} \\
k_{tn} & k_{nn}
\end{bmatrix} = \begin{bmatrix}
-\hat{n}_y & \hat{n}_x \\
\hat{n}_x & \hat{n}_y
\end{bmatrix} \begin{bmatrix}
k_{11} & 0 \\
0 & k_{22}
\end{bmatrix} \begin{bmatrix}
-\hat{n}_y & \hat{n}_x \\
\hat{n}_x & \hat{n}_y
\end{bmatrix} = \begin{bmatrix}
k_{11}\hat{n}_y^2 + k_{22}\hat{n}_x^2 & -k_{11}\hat{n}_x\hat{n}_y + k_{22}\hat{n}_x\hat{n}_y \\
-\hat{n}_y^2 & \hat{n}_x^2 + k_{22}\hat{n}_x\hat{n}_y
\end{bmatrix} \text{sym}
\]  

(11)

where subscripts 1 and 2 denote the directions of material orientation and \( \hat{n}_x \) and \( \hat{n}_y \) are the components of the normal unit vector in the local system. If isotropic material is considered \( k_{11} = k_{22} = k \) and being \( \hat{n}_x^2 + \hat{n}_y^2 = 1 \) one get:

\[
k^{t-n}_{iso} = \begin{bmatrix}
k & 0 \\
0 & k
\end{bmatrix}
\]  

(12)

It is worth noting that for isotropic material the classical definition of flux applies, i.e. it is normal to the isothermal surface passing through the spatial position considered. This is easy to verify from the previous equations, because when an isothermal surface is considered \( \partial \theta / \partial t = 0 \) and, according to Eq. (9) and (12), the only component of flux different from zero is \( q_n \).

One may notice that with this model of interface conductivity, the thermal conductance \( h_c \) has been neglected. This is usually responsible for a temperature drop between two surfaces.
in contact and it could be considered and easily implemented in Eq. (7) as an additional resistance which usually depends on the roughness of the surfaces, the contact pressure or presence of interstitial impurities. In this model however the the difference of temperature between the two surfaces of the interface depends only on the level of damage and for a pristine interface between $A$ and $B$ the condition $\theta_A = \theta_B$ is enforced.

3. Thermoelasticity equations

3.1. Overview

The most general thermoelastic problems are governed by the equation of motion (Navier-Cauchy equation) and the heat conduction equation. Here the equations for linear, elastic, isotropic and homogeneous body occupying a domain $V$ enclosed by a boundary $S$ are represented by:

\[
\begin{aligned}
\mu u_{i,\text{jj}} + \frac{\mu}{(1 - 2\nu)} u_{j,\text{ii}} - \frac{2\mu(1 + \nu)}{(1 - 2\nu)} \alpha \theta_{,i} - \rho \ddot{u}_i + \psi_i &= 0 \\
\lambda \theta_{,ii} &= \theta_0 \\
\end{aligned}
\]

(13)

where $\theta$ is the temperature, $u$ is the displacement, $\mu$ is the shear modulus, $\nu$ is the Poisson’s ratio and $\alpha$ is the coefficient of thermal expansion. The notation $(\cdot)_{,i}$ stands for differentiation with respect to the $i$th spatial coordinate and Einstein notation applies. The heat flux is defined as $q = -k\theta_{,i}$ where $k$ is the thermal conductivity, coherently with Eq. (4).

In order to obtain the solution to Eq. (13) for the determination of temperature, fluxes, displacements and tractions in polycrystalline aggregates, in this work the boundary element method has been used. Due to the nature of the domain under examination, a multi-region and dual-boundary element formulation needs to be considered. Since the formulation dealing with the transition between intergranular and transgranular damage has been extensively covered in [1], here the final set of equations is reported and more attention is focused on the thermoelastic aspects. For the sake of clarity let us consider a generic polycrystalline aggregate as shown in Figure 2 where the surfaces of each grain $H = 1 \ldots N_g$ can be classified as: non-contact ($S_{\text{nc}}^H$) resulting from the intersection between grains and the outer domain’s boundary, contact ($S_{\text{c}}^H$) which are the interfaces between adjacent grains, and transgranular coplanar surfaces ($S_{\text{cr}}^{H+}$, $S_{\text{cr}}^{H-}$). The following relationships apply [1]:

\[
S_*^H = S_{\text{nc}}^H \cup S_{\text{c}}^H \quad ; \quad S^H = S_*^H \cup (S_{\text{cr}}^{H+} \cup S_{\text{cr}}^{H-})
\]

(14)

Following Prasad and Aliabadi [30, 31], the boundary integral equations involved in the solution of the problem are the Displacement, Traction, Temperature and Flux equations.
In this work however not only is the problem formulated in terms of opening displacements of the transgranular interfaces ($\delta u_{cr}$) but also in terms of temperature jumps ($\delta \theta_{cr}$); this choice is helpful since a cohesive thermo-mechanical approach has been used, so that tractions and opening displacements are related as well as fluxes and temperature jumps. With this premises, when the mechanical and the thermal problems are solved together for numerical convenience (even though it is an uncoupled problem), the system of equations to solve is composed by:

- Displacement equation for collocation on $S^H$
- Traction equation for collocation on $S^H_{cr}$
- Temperature equation for collocation on $S^H$
- Temperature equation for collocation on $S^H_{cr}$
- Flux equation for collocation on $S^H_{cr}$

It is worth noting that although the dual BEM has been used, an additional temperature equation for collocation on the transgranular elements is needed. For the pure thermal problem then, the only flux equation would be sufficient for collocation on transgranular elements, but the actual temperature of the crack would be still unknown. However the traction equation cannot be expressed only in terms of the temperature difference across the crack, but both temperatures are required or one temperature and the difference. In other words the mechanical solutions to two thermo-elastic problems having the same crack’s
temperature jump but different actual temperatures (e.g. $\theta_1^{cr+} = 5^\circ C$, $\theta_1^{cr-} = 10^\circ C$ and $\theta_2^{cr+} = 20^\circ C$, $\theta_2^{cr-} = 205^\circ C$) are different, as intuitively understandable. If instead the thermal problem was solved separately an additional temperature equation would be required anyway in post-processing to retrieve the temperature of one of the crack’s surfaces.

3.2. Steady-state

Depending on the application and the material into consideration some simplifications apply. If the inertial term is neglected from the motion equation as well as the strain rate from the heat equation and the diffusive processes are considered completed, the two equations of uncoupled steady-state thermoelasticity can be expressed as follows:

$$\begin{cases} 
\mu u_{i,jj} + \frac{\mu}{(1-2\nu)} u_{j,ji} + \psi_i = \frac{2\mu(1+\nu)}{(1-2\nu)} \alpha \theta, \\
\theta,_{ii} = 0
\end{cases} \quad (15)$$

The boundary integral equations are written below, where fundamental solutions related to opposite coplanar surfaces have been simplified already for the sake of brevity, and interface boundary conditions on cracks have been applied, as

$$\begin{cases} 
\delta \tilde{u}(x,cr) = \tilde{u}(x^+) + \tilde{u}(x^-) \\
\tilde{t}(x,cr) = \tilde{t}(x^+) = \tilde{t}(x^-)
\end{cases} ; \begin{cases} 
\delta \theta(x,cr) = \theta(x^+) - \theta(x^-) \\
q(x,cr) = q(x^+) = -q(x^-)
\end{cases} \quad (16)$$

Displacement Equation

$$C^H_{ij}(x') \tilde{u}^H_j(x') = \int_{\tilde{S}^H} \tilde{U}^H_{ij}(x', x) \tilde{u}^H_j(x) d\tilde{S}^H + \int_{\tilde{S}^H} \tilde{T}^H_{ij}(x', x) \delta \tilde{u}^H_j(x) d\tilde{S}^H + \int_{\tilde{S}^H} P^H_i(x', x) \delta \theta(x) d\tilde{S}^H + \int_{\tilde{S}^H} Q^H_i(x', x) q^H(x) d\tilde{S}^H + (17)$$

where $\tilde{f}$ stands for Cauchy principal value integral and $P_i$ and $Q_i$ come from the transformation of a volume integral, using the Galerkin vector and the condition $\theta,_{ii} = 0$ [10].
The set of equations (17–21), for each grain

\[ t_j^H(x'_{cr}) = \hat{n}_i(x^+) \int_{S^H} \hat{D}_{kij}^H(x^+, x)\hat{J}_k^H(x) d\hat{S}_*^H - \hat{n}_i(x^+) \int_{S^H} \hat{S}_{kij}^H(x^+, x)\hat{u}_k^H(x) d\hat{S}_*^H + \]

\[ -\hat{n}_i(x^+) \int_{\bar{S}^H} \hat{S}_{kij}^H(x^+, x_{cr})\delta\hat{u}_k^H(x_{cr}) d\bar{S}_{cr}^H + \hat{n}_i(x^+) \int_{\bar{S}^H} \hat{P}_{ij}^H(x^+, x)\theta^H(x) d\bar{S}_{cr}^H + \]

\[ +\hat{n}_i(x^+) \int_{\bar{S}^H} \hat{P}_{ij}^H(x^+, x_{cr})\delta\theta^H(x_{cr}) d\bar{S}_{cr}^H - \hat{n}_i(x^+) \int_{\bar{S}^H} \hat{Q}_{ij}^H(x^+, x)q^H(x) d\bar{S}_{cr}^H + \]

\[ -\hat{n}_i(x^+) \frac{E\alpha}{1 - 2\nu} \delta_{ij}\theta^H(x_{cr}) + \hat{n}_i(x^+) \frac{E\alpha}{2(1 - 2\nu)} \delta_{ij}\delta\theta^H(x_{cr}) \]

where \( \hat{f} \) stands for Hadamard finite part integral.

Temperature Equations

\[ C^H (x')\theta^H (x') = \int_{S^H} q^{\nu^H} (x', x)\theta(x) d\hat{S}_*^H - \int_{S^H} \theta^{\nu^H} (x', x)q(x) d\hat{S}_*^H + \]

\[ + \int_{\bar{S}^H} q^{\nu^H} (x', x_{cr})\theta(x_{cr}) d\bar{S}_{cr}^H \]

\[ \theta^H(x'_{cr}) - \frac{1}{2}\delta\theta^H(x'_{cr}) = \int_{S^H} q^{\nu^H} (x^+, x)\theta(x) d\hat{S}_*^H - \int_{S^H} \theta^{\nu^H} (x^+, x)q(x) d\hat{S}_*^H + \]

\[ + \int_{\bar{S}^H} q^{\nu^H} (x^+, x_{cr})\theta(x_{cr}) d\bar{S}_{cr}^H \]

Flux Equation

\[ q^H(x'_{cr}) = \hat{n}_i(x^+) \int_{S^H} \theta^{\nu^H} (x^+, x)q^H(x) d\hat{S}_*^H - \hat{n}_i(x^+) \int_{S^H} q^{\nu^H} (x^+, x)\theta^H(x) d\hat{S}_*^H + \]

\[ -\hat{n}_i(x^+) \int_{\bar{S}^H} q^{\nu^H} (x^+, x_{cr})\theta^H(x_{cr}) d\bar{S}_{cr}^H \]

Details about the integrals’ kernels used in the above equations are shown in Appendix A.1

The set of equations \([17, 21]\), for each grain \( H = 1, \ldots, N_g \), can be written in matrix form as
follows:

\[
\begin{bmatrix}
\hat{H}^d & \hat{H}^d_{\theta cr} & H^d_{\theta cr} & 0 & H^d_{\theta cr} \\
\hat{H}^t & \hat{H}^t_{\theta cr} & H^t_{\theta cr} & 0 & H^t_{\theta cr} \\
0 & 0 & H^t_{\theta cr} & 0 & H^t_{\theta cr} \\
0 & 0 & H^q_{\theta cr} & 0 & H^q_{\theta cr}
\end{bmatrix}
\begin{bmatrix}
\tilde{\mathbf{u}} \\
\tilde{\mathbf{u}}_{\theta cr} \\
\delta \tilde{\mathbf{u}}_{\theta cr} \\
\delta \tilde{\mathbf{t}}_{\theta cr}
\end{bmatrix}
= 
\begin{bmatrix}
\tilde{\mathbf{G}}^d & 0 & G^d_{\theta} & 0 \\
\tilde{\mathbf{G}}^t & I & G^t_{\theta} & 0 \\
0 & 0 & G^t_{\theta cr} & 0 \\
0 & 0 & G^q_{\theta cr} & G^q_{\theta cr}
\end{bmatrix}
\begin{bmatrix}
\tilde{\mathbf{t}} \\
\tilde{\mathbf{t}}_{\theta cr} \\
\delta \tilde{\mathbf{t}}_{\theta cr} \\
\delta \mathbf{q}_{cr}
\end{bmatrix}
\] (22)

where the superscripts \(d, t, \theta, \theta_{cr}\) and \(q\) stand for displacement, traction, temperature, temperature on crack and flux equation respectively; \(c = \frac{E_0}{2(1-2\nu)}\) is the additional term in the traction equation due to thermal strains \(\varepsilon_{ij}^{mech} = \varepsilon_{ij}^{tot} - \varepsilon_{ij}^{\theta} \delta_{ij}\) and plane strain assumption \(\varepsilon_{zz}^{tot} = \varepsilon_{xz} = \varepsilon_{yz} = 0\). \(\mathbf{I}\) is an identity sub-matrix and \(\mathbf{0}\) a null sub-matrix. \(\tilde{\mathbf{u}}\) and \(\tilde{\mathbf{t}}\) contain known and unknown values of displacements and tractions respectively on contact and non-contact surfaces, \(\delta \tilde{\mathbf{u}}_{\theta cr}\) and \(\delta \tilde{\mathbf{t}}_{\theta cr}\) contain unknown values of jump displacements and tractions respectively on the transgranular surfaces. \(\mathbf{\theta}\) and \(\mathbf{q}\) contain known and unknown values of temperatures and fluxes respectively on contact and non-contact surfaces; \(\theta_{cr}, \mathbf{q}_{cr}\) and \(\delta \theta_{cr}\) contain respectively unknown values of temperature, fluxes and temperature difference across the transgranular surface. The symbol \(\tilde{\cdot}\) refers to a field in the reference system of the local surface, in terms of tangential and normal directions (see Appendix [B]).

After applying the boundary condition and re-arranging the matrices, the system can be expressed as in Eq. (23). This final matrix has been written for two generic \(n^{th}\) and \(m^{th}\) grains sharing an interface; this has been done to highlight how the system of matrix is rearranged and how interface boundary conditions are applied to the system. The field variables have been divided into known and unknown vectors: \(\mathbf{x}\) and \(\mathbf{x}_{\theta}\) contain mixed terms respectively of unknown displacement or tractions and temperatures or fluxes on the outer boundary \(S_{nc}\); \(\tilde{\mathbf{y}}\) and \(\mathbf{y}_{\theta}\) contain known values of the aforementioned fields, applied through the boundary conditions (BC). Sub-matrices \(\mathbf{A}\) and \(\mathbf{B}\) contain mixed component of \(\mathbf{H}\) and \(\mathbf{G}\) and sub-matrices \(\Phi\) contain the cohesive laws relating \(\delta \mathbf{u}\) to \(\mathbf{t}\) and \(\delta \theta\) to \(\mathbf{q}\). Moreover the right hand side has been divided into two vectors, one containing only mechanical variables \((\mathbf{F}^m)\) and the other only thermal variables \((\mathbf{F}^\theta)\); this helps in applying different loading factors to the mechanical or the thermal boundary conditions during the incremental loading procedure.
\[
\begin{bmatrix}
A^m_{\theta} A^m_{\theta} & \tilde{H}_{\theta I}^m & 0 & \tilde{G}_{\theta I}^m & 0 & H_{\theta I}^m & 0 & 0 & -G_{\theta I}^m & 0 \\
A^m_{\theta} A^m_{\theta} & \tilde{H}_{\theta I}^m & 0 & \tilde{G}_{\theta I}^m & I & H_{\theta I}^m & 2eI & 0 & c I + H_{\theta I}^m & -G_{\theta I}^m \\
0 & A^m_{\theta} & 0 & 0 & 0 & 0 & H_{\theta I}^m & 0 & H_{\theta I}^m & -G_{\theta I}^m \\
0 & A^m_{\theta} & 0 & 0 & 0 & 0 & H_{\theta I}^m & 0 & -H_{\theta I}^m & -G_{\theta I}^m \\
0 & A^m_{\theta} & 0 & 0 & 0 & 0 & H_{\theta I}^m & 0 & H_{\theta I}^m & -G_{\theta I}^m \\
\end{bmatrix}
\begin{bmatrix}
\dot{x} \\
\dot{x}_{\theta} \\
\dot{u}^I \\
\delta \dot{u}^I \\
\dot{t}^c \\
\theta_I \\
\theta_{cr} \\
\delta \theta_I \\
\delta \theta_{cr} \\
q^I \\
q_{cr} \\
\end{bmatrix}
= \begin{bmatrix}
\dot{B}_{\theta}^m & \ddot{y} \\
\ddot{B}_{\theta}^m & \ddot{y} \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
\end{bmatrix} + \begin{bmatrix}
B_{\theta}^m & y_{\theta} \\
B_{\theta}^m & y_{\theta} \\
B_{\theta}^m & y_{\theta} \\
B_{\theta}^m & y_{\theta} \\
B_{\theta}^m & y_{\theta} \\
\end{bmatrix}
\begin{bmatrix}
\phi_I \\
\phi_{cr} \\
\phi_I \\
\phi_{cr} \\
\phi_I \\
\phi_{cr} \\
\phi_I \\
\phi_{cr} \\
\phi_I \\
\phi_{cr} \\
\phi_I \\
\phi_{cr} \\
\end{bmatrix}
\]

(23)
3.3. Transient

If thermoelastic problems need to be studied in presence of diffusive phenomena, uncoupled transient thermoelastic equations can be expressed as:

\[
\begin{aligned}
\mu u_{i,ij} + \frac{\mu}{(1-2\nu)} u_{j,ji} + \psi_i &= \frac{2\mu(1+\nu)}{(1-2\nu)} \alpha \theta_j \\
\theta_{ji} - \frac{1}{\kappa} \dot{\theta} &= 0
\end{aligned}
\]  

(24)

where \( \kappa = k / c_t \) is the thermal diffusivity, \( k \) is the thermal conductivity and \( c_t \) is the heat capacity per unit volume at constant strain. Below the boundary integral equations are written, and relationships in Eq. (16) apply again.

Displacement Equation

\[
C^{H}_{ij}(x') \dot{u}^{H}_{j}(x' , \tau_F) = \int_{S_{H}^{F}} \tilde{U}^{H}_{ij}(x', x) \tilde{u}^{H}_{j}(x, \tau_F) d\tilde{S}_{x}^{H} - \int_{S_{H}^{F}} \tilde{T}^{H}_{ij}(x', x) \tilde{u}^{H}_{j}(x, \tau_F) d\tilde{S}_{x}^{H} + \\
- \int_{S_{H}^{F}} \tilde{T}^{H}_{ij}(x', x_{cr}) \delta \tilde{u}^{H}_{j}(x_{cr}, \tau_F) d\tilde{S}_{cr}^{H} - \int_{S_{H}^{F}} \int_{\tau_0}^{\tau_F} F^{H}_{i}(x', x, \tau_F, \tau) \delta H(x, \tau) d\tau d\tilde{S}_{x}^{H} + \\
- \int_{S_{H}^{F}} \int_{\tau_0}^{\tau_F} F^{H}_{i}(x', x_{cr}, \tau_F, \tau) \delta H(x_{cr}, \tau) d\tau d\tilde{S}_{cr}^{H} + \int_{S_{H}^{F}} \int_{\tau_0}^{\tau_F} G^{H}_{ij}(x', x, \tau_F, \tau) q^{H}(x, \tau) d\tau d\tilde{S}_{x}^{H}
\]  

(25)

Traction Equation

\[
\tilde{\sigma}^{H}_{j}(x'_{cr}, \tau_F) = \dot{\bar{n}}_{i}(x'^{+}) \int_{S_{H}^{F}} \tilde{D}^{H}_{kij}(x'^{+}, x) \tilde{\sigma}^{H}_{k}(x, \tau_F) d\tilde{S}_{x}^{H} - \dot{\bar{n}}_{i}(x'^{+}) \int_{S_{H}^{F}} \tilde{D}^{H}_{kij}(x^{+}, x) \tilde{\sigma}^{H}_{k}(x, \tau_F) d\tilde{S}_{x}^{H} + \\
- \dot{\bar{n}}_{i}(x'^{+}) \int_{S_{H}^{F}} \tilde{D}^{H}_{kij}(x^{+}, x_{cr}) \delta \tilde{\sigma}^{H}_{k}(x_{cr}, \tau_F) d\tilde{S}_{cr}^{H} - \dot{\bar{n}}_{i}(x'^{+}) \int_{S_{H}^{F}} \int_{\tau_0}^{\tau_F} \tilde{D}^{H}_{ij}(x'^{+}, x, \tau_F, \tau) \delta H(x, \tau) d\tau d\tilde{S}_{x}^{H} + \\
- \dot{\bar{n}}_{i}(x'^{+}) \int_{S_{H}^{F}} \int_{\tau_0}^{\tau_F} \tilde{D}^{H}_{ij}(x'^{+}, x_{cr}, \tau_F, \tau) \delta H(x_{cr}, \tau) d\tau d\tilde{S}_{cr}^{H} + \\
+ \dot{\bar{n}}_{i}(x'^{+}) \int_{S_{H}^{F}} \int_{\tau_0}^{\tau_F} \tilde{D}^{H}_{ij}(x'^{+}, x, \tau_F, \tau) q^{H}(x, \tau) d\tau d\tilde{S}_{x}^{H} - \dot{\bar{n}}_{i}(x'^{+}) \frac{E\alpha}{1-2\nu} \delta_{ij} \theta^{H}(x_{cr}, \tau_F) + \\
+ \dot{\bar{n}}_{i}(x'^{+}) \frac{E\alpha}{2(1-2\nu)} \delta_{ij} \theta^{H}(x_{cr}, \tau_F)
\]  

(26)
Temperature Equations

\[ C^H(x') \theta^H(x', \tau_F) = \int_{\tilde{S}_F} \int_{\tau_0}^{\tau_F} Q^H(x', x, \tau_F, \tau) \theta(x, \tau) d\tau d\tilde{S}_s^H + \]
\[ - \int_{\tilde{S}_F} \int_{\tau_0}^{\tau_F} \Theta^H(x', x, \tau_F, \tau) q(x, \tau) d\tau d\tilde{S}_s^H + \int_{\tilde{S}_F} \int_{\tau_0}^{\tau_F} Q^H(x', x_{cr}, \tau_F, \tau) \theta(x_{cr}, \tau) d\tau d\tilde{S}_{cr}^H \]
\[ \theta^H(x_{cr}, \tau_F) - \frac{1}{2} \delta \theta^H(x_{cr}, \tau_F) = \int_{\tilde{S}_F} \int_{\tau_0}^{\tau_F} Q^H(x^+, x, \tau_F, \tau) \theta(x, \tau) d\tau d\tilde{S}_s^H + \int_{\tilde{S}_F} \int_{\tau_0}^{\tau_F} Q^H(x^+, x_{cr}, \tau_F, \tau) \theta(x_{cr}, \tau) d\tau d\tilde{S}_{cr}^H \]

Flux Equation

\[ q^H(x'_{cr}, \tau_F) = \bar{n}_i(x^+) \int_{\tilde{S}_F} \int_{\tau_0}^{\tau_F} \Theta^{**}(x^+, x, \tau_F, \tau) q^H(x, \tau) d\tau d\tilde{S}_s^H + \]
\[ - \bar{n}_i(x^+) \int_{\tilde{S}_F} \int_{\tau_0}^{\tau_F} Q^{**}(x^+, x, \tau_F, \tau) \theta^H(x, \tau) d\tau d\tilde{S}_s^H + \int_{\tilde{S}_F} \int_{\tau_0}^{\tau_F} Q^{**}(x^+, x_{cr}, \tau_F, \tau) \theta^H(x_{cr}, \tau) d\tau d\tilde{S}_{cr}^H \]

3.3.1. Time Integration

The components relative to a thermal variable (Eq. 25-29) require temporal and spatial integration. Time integration is done analytically and the spatial integration of constant elements is evaluated either analytically or numerically depending on the location of the elements. The time domain \((\tau_0 \text{ to } \tau_F)\) is divided into \(F\) time steps of equal size \(\Delta \tau\). Constant or linear time interpolation can be chosen, however the former has been proven inaccurate with the use of the flux equation [31]. The time function inside the generic \(f^{th}\) time step can be written as:

\[ \tau = M^b \tau^b \quad \left[ \tau_{f-1} \leq \tau \leq \tau_f \right] \]

where \(\tau^b\) are the temporal nodes and \(M^b\) are the shape functions for the linear time interpolation:

\[ M^b = \left[ \frac{\tau_f - \tau}{\Delta \tau}, \frac{\tau - \tau_{f-1}}{\Delta \tau} \right] \]
The generic term with a time integral in equations (25-29) can be rewritten in a discretized form as:

$$\int_{\Gamma} \int_{\tau_0}^{\tau_F} Q(x', x, \tau_F, \tau) \theta(x, \tau) d\tau d\Gamma = \sum_{n=1}^{N} \left[ \int_{\Gamma_n} \left\{ \sum_{f=1}^{F} \int_{\tau_{f-1}}^{\tau_f} QM^b d\tau \right\} d\Gamma \right] \theta^{bf}_{n f}$$ (32)

Details of the temporal integration of the fundamental solutions used in Eq. (25) and (29) are shown in Appendix A.2. In compact matrix form the temperature equation can be written as:

$$\sum_{i,j=1}^{N} \sum_{f=1}^{F} \left( H^1_{ijFf} \theta_{j(f-1)} + H^2_{ijFf} \theta_{i f} \right) = \sum_{i,j=1}^{N} \sum_{f=1}^{F} \left( G^1_{ijFf} q_{j(f-1)} + G^2_{ijFf} q_{i f} \right)$$ (33)

where

$$H_{ijFf} = \hat{H}_{ijFf} + C_i \delta_{ij} \delta_{Ff}$$ (34)

In (33), the subscripts denote collocation element \((i)\), integration element \((j)\), current “collocation” time step \((F)\) and “integration” time step \((f)\). When collocating on all the spatial elements, the system can be rewritten as:

$$\sum_{f=1}^{F} \left( H^1_{Ff} \theta_{f-1} + H^2_{Ff} \theta_{f} \right) = \sum_{f=1}^{F} \left( G^1_{Ff} q_{f-1} + G^2_{Ff} q_{f} \right)$$ (35)

or

$$H^2_{Ff} \theta_{F} = G^2_{Ff} q_{F} + S_F$$ (36)

where the second temporal node of the current time step has been separated from what represents instead the time history of each element. This procedure for time integration leads to an additional right hand side vector \(S_F\) which contains the information of all the previous time steps.

$$S_F = - \sum_{f=1}^{F} \left( H^1_{Ff} \theta_{f-1} + H^2_{Ff} \theta_{f} \right) - H^1_{F_F} \theta_{F-1} + \sum_{f=1}^{F} \left( G^1_{Ff} q_{f-1} + G^2_{Ff} q_{f} \right) + G^1_{F_F} q_{F-1}$$ (37)

The same approach applies to the terms of the other equations having a time integral. From a numerical point of view this requires the calculation of new integrals at every new time step, but if constant \(\Delta \tau\) are chosen, since the actual time variable in all the fundamental solutions is \((\tau_F - \tau_f)\), at every new step \(F\), only \(H_{F1}\) and \(G_{F1}\) have to be evaluated because...
\[ H_{FF} = H_{11} = \cdots = H_{ff}, \quad H_{F(F-1)} = H_{21} = \cdots = H_{f(f-1)} \text{ and so on; the same applies for G and all the other time steps.} \]

Equation (23) can be then written in compact form for transient formulation as:

\[
\begin{bmatrix}
\tilde{A}_{nc} & \tilde{A}_c & \tilde{A}_{\theta c} \\
0 & \Phi & 0 \\
0 & 0 & \Phi_\theta
\end{bmatrix}
\begin{bmatrix}
\tilde{x} \\
\tilde{x}_\theta \\
\tilde{U}_I \\
\delta\tilde{U}_I \\
\delta\tilde{U}^{cr}_I \\
\tilde{T}_I \\
\theta_I \\
\theta^{cr}_I \\
\delta\theta_I \\
\delta\theta^{cr}_I \\
q_I \\
q^{cr}_I
\end{bmatrix} = F^m + F^\theta + S_F
\]

where \( A \) and \( F \) contain mixed terms of \( H \) and \( G \) but evaluated at the second temporal node of the current time step and \( S_F \) represents the memory of the previous time steps.

### 3.4. Transient/Steady-State Transition

From a physical point of view not only does the choice to use a steady-state rather than a transient approach depend on the behaviour that needs to be modelled, but it also depends on relative time-scales of thermal and elastic phenomena for the material and application under examination. In this work the development of the mechanical behaviour has been considered quasi-static, following the iterative loading procedure explained in [1]. For the steady-state formulation (Section 3.2), the same procedure has been applied to the thermal boundary conditions, with the possibility to assign different loading factors (\( \lambda \) and \( \lambda^\theta \)) and loading rates to mechanical and thermal loading. In the transient formulation however, after choosing a time range, the system in Eq. (38) is solved at every time step and the thermo-mechanical solution is updated until convergence to the steady-state regime is reached. At this point the thermal transitory is completed but the mechanical loading can be further increased quasi-statically. It is for this reason that in this work the two formulations, presented respectively in Sections 3.2 and 3.3, have been linked upon transient convergence. From a numerical point of view this is very convenient because updating and solving the system in Eq. (38) requires extra memory which is necessary to store the additional vector \( S_F \). Instead the
sub-matrices \( \Phi \) on the left hand side, containing up to date information about the cohesive status of the interfaces/cracks are saved and the sub-matrices \( A \) and \( B \) are re-evaluated using the time-independent fundamental solutions of the steady state formulation; the new thermal boundary condition are applied coherently to the last solution of the transient formulation on all the elements, so the vector \( S_F \) is no more required and even new mechanical BC can be applied. This approach has been proved, during the development of the current model, to produce the same results of the fully transient formulation but with the advantage of being less computationally expensive and more straightforward after transitory convergence.

4. Results and investigations

In this section the numerical simulations performed using the proposed formulations are presented: a few examples have been analysed with the aim to validate the method developed here and investigate some physical behaviours of the materials and the microstructures under examination in this work. Comparisons to literature and finite element results will be also presented.

4.1. Steady-state

Introduction

To validate the steady-state formulation some literature examples showing crack propagation in homogeneous structures with thermal and mechanical loads have been reproduced and proved in good agreement with the crack patterns obtained on literature \[30\]. Here one of these examples is presented, in which not only is the crack pattern of a rectangular homogeneous plate under the effect of thermo-mechanical loading obtained, but it is also compared to the (inter- and trans-granular) crack path exhibited by the equivalent structure obtained as a multi-grain aggregate (Figure 3). The plate has an initial crack at the left edge, whose length is defined by \( a/w = 0.5 \) where \( w = h = 0.5 \), and the angle with the vertical axes is \( \alpha = 45^\circ \). The material considered is isotropic with Young’s modulus \( E = 218400 \) MPa, Poisson’s ratio \( \nu = 0.3 \) and coefficient of thermal expansion \( \alpha = 1.67 \times 10^{-5} / ^\circ C \). The top edge (\( AB \)) is considered at a temperature \( \theta^{AB} = -20^\circ C \) and the bottom edge (\( CD \)) at a temperature \( \theta^{CD} = 20^\circ C \); vertical displacements at the bottom edge have been constrained (\( u_y^{CD} = 0 \)) and tensile traction has been enforced on the top edge (\( t_y^{AB} = 10 \) Pa). This comparison shows very good agreement between the homogeneous and the polycrystalline case, in which the intergranular and transgranular damage follows the macroscopic crack pattern.

Next, the effect of thermal loading on different polycrystalline microstructures will be shown. It is well known that many ceramic materials can experience damage or cracking when cooled from high processing temperatures. In the following simulations this behaviour
Figure 3: Comparison between macro and micro crack paths for slant edge crack, under the action of thermo-mechanical load.

has been investigated. The polycrystalline material under examination is an aggregate of 

alumina (Al\textsubscript{2}O\textsubscript{3}) and silicon carbide (SiC), whose material properties are shown in Table 1

An interesting parameter for a first analysis of damage measurement is introduced here, following Sridar et al [8]:

\[
\rho_c = \sum_{i=1}^{N_{int}} \frac{2L_i}{L_{int}} \quad [0 \leq \rho_c \leq 1] \quad (39)
\]
Here the parameter \( \rho_c \) expresses the cumulative length of interfaces experiencing damage as a fraction of the total interfaces’ length. Thus \( N_{\text{int}} \) is the number of interfaces (including transgranular ones), \( L_i \) and \( d(i) \) are respectively the semi-length and damage level of the \( i^{th} \) element, as in [3], and \( L_{\text{int}} \) is the total length of the microstructure’s interfaces. Hence the problem here has been studied in terms of cohesive damage instead of broken bonds, as in [5].

However the parameter \( \rho_c \) does not provide information on the level of damage and degradation of the microstructure, i.e. on the residual strength of the material. So here another additional parameter to describe the damage process has been chosen: in the framework of multi-scale analysis, since we are dealing with micro-structures, the damage parameter \( D \) needs to be introduced. For every loading step the total average stress can be evaluated by means of averaging theorems [41]; the volume average of stresses over a volume \( V \) of a microstructure, using the divergence theorem, is given by:

\[
\bar{\sigma}_{ij} = \frac{1}{V} \int_V \sigma_{ij} dV = \frac{1}{V} \int_S x_i t_j dS
\]  

(40)

where \( x_i \) is the \( i^{th} \) component of the position vector of the point lying on the external boundary \( (S) \).

The strains can be evaluated instead as follows, where again the divergence theorem has been applied:

\[
\bar{\varepsilon}_{ij} = \frac{1}{2V} \int_V (u_{i,j} + u_{j,i}) dV = \frac{1}{2V} \int_S (u_i n_j + u_j n_i) dS
\]  

(41)

It is interesting to highlight here that in the case of cohesive cracks or internal discontinuities, the average stress is not affected because they are either in equilibrium or traction free and the integral (40) is evaluated only along the external boundary of the domain. The same simplification does not apply however to the strains, therefore internal discontinuities or decohesions have to be considered explicitly in (41) due to the local displacement jumps \( \delta u_i^l \). Hence the more general relationship applies:

\[
\bar{\varepsilon}_{ij} = \frac{1}{2V} \left\{ \int_S (u_i n_j + u_j n_i) dS - \int_{S^l} (\delta u_i^l n_j^l + \delta u_j^l n_i^l) dS^l \right\}
\]  

(42)

where \( S^l \) are the surfaces of the discontinuities and \( n_i^l \) the components of their unit normal vectors.

The overall decremental stress is then defined as [42]:

\[
\bar{\sigma}^D = \sigma^e - \bar{\sigma}^t
\]  

(43)
where $\sigma^e$ is the elastic stress obtained in absence of any micro-damage and $\bar{\sigma}^t$ is the actual overall stress evaluated using Eq. (40). Then

$$\sigma^D_{ij} = D_{ij}C_{ijkl}(\varepsilon_{kl}^{\text{tot}} - \varepsilon_{kl}^{\theta} \delta_{kl}) = D_{ij} \sigma^e_{ij}$$

Hence in virtue of Eq. (43) and (44):

$$D = 1 - \bar{\sigma}^t |\sigma^e|^{-1}$$

From Eq. (45) it is interesting to note that depending on the loading condition and then on the direction of damage propagation, the overall effect could be the loss of “macro-isotropy” of the aggregate: if the macro-damage evolves in $y$ direction due to any load along the $x$ axes, the main softening of the microstructure will occur in the $x$ direction and hence the predominant decremental damage component will be $D_{11}$. 

For the sake of completeness, an investigation into the effect of the presence of additional phases in the aggregate has been done in this work, comparing alumina microstructures with different percentages of silicon carbide. As mentioned in the introduction, the effect on grain refinement has been neglected here, so only the strengthening effect of the additional phase is expected. Figure 4 shows the damage $D$ as a function of the thermal load applied to three microstructures with same grain size ($d_{gr} = 3.34 \mu m$) and morphology, but different silicon carbide presence: 0%, 10% and 50%. Displacements have been constrained at two opposite edges and the other two have been considered traction free; thermal loading has been applied quasi-statically until failure. It is evident from Figure 4 that the damage level for a given thermal load is lower as the presence of SiC increases, thus the additional presence of the second phase improves the damage and degradation process; these results are in good qualitative agreement with the literature results [36]. In the next simulations the volume presence of the two phases has been considered 50% and they have been distributed randomly across the aggregate. For the sake of statistical relevance, these and the following results have been obtained by averaging the outcomes of three sets of simulations on different morphologies.

4.1.1. Unconstrained micro-structures

Here, the first set of simulations aims to investigate the effect of grain size on damage behaviour due to thermal load in unconstrained microstructure. It is worth highlighting again here that in single-phase isotropic materials loaded quasi-statically there would be no mechanism causing stress generation and consequently damage onset. However the mismatch of thermal expansion/contraction between different phases, represents here the cause of
Figure 4: Damage $D$ as a function of the thermal load $\Delta \theta$ for different percentages of SiC presence in the microstructure.

Figure 5: Microstructures with different grain sizes.

Damage generation, and it is generally called spontaneous cracking. Figure 5 shows three of the microstructures on which the simulations have been performed; grain size has been defined according to ASTM E112 – 13: 30 grains with an average grain size $G = 11.7$ ($\bar{A}_{gr} = 37.17 \mu m^2$, $\bar{d}_{gr} = 6.1 \mu m$), 50 grains with $G = 12.5$ ($\bar{A}_{gr} = 22.3 \mu m^2$, $\bar{d}_{gr} = 4.72 \mu m$) and 100 grains with $G = 13.5$ ($\bar{A}_{gr} = 11.15 \mu m^2$, $\bar{d}_{gr} = 3.34 \mu m$); in all the cases the side length of the square microstructure is $l = 33.39 \mu m$.

The microstructures’ edges have not been constrained (only rigid motion has been suppressed), so that the overall aggregates could expand or contract freely; uniform thermal load
\(\Delta \theta\) has been applied quasi-statically, by means of a loading factor (as mentioned in Section 3.2), until the desired deformation or damage level has been reached.

Initially weak grains’ boundaries are considered where the ratio between critical fracture energy of grains’ boundaries and grains’ interior \(R = G_{\text{inter}}/G_{\text{trans}} < 1\). A ratio \(R = 0.7\) has been chosen here because simulations under uni-axial tension have shown to be the minimum value for which intergranular-transgranular transition happens, but without critical transgranular damage, for the grain morphology considered \[1\]. These first results are then purely intergranular.

Figure 6(a) shows \(\rho_c\) as a function of the thermal load applied to the different microstructures and Figure 7 shows the damaged interfaces within the aggregates. As a general trend it is easy to notice that microstructures with finer grains exhibit more damage under the action of the same thermal load, and it increases as the load increases. However it is interesting to notice what happens at low temperatures when the onset of damage occurs in the three microstructures: the insert in the figure shows the early stage of the simulation and it is evident that the trend here is inverted, i.e. when the same thermal load is considered for the three aggregates, coarse grain structure exhibits higher level of damage than finer grains. These results can be compared qualitatively to the ones obtained by Sridhar et al in \[8\]. Even though in their simulations they considered anisotropic thermal expansion, here, at least at a micro-mechanical level, the mechanism causing damage onset is the same, i.e. thermal expansion mismatch. In \[8\] the same overall behaviour has been captured when the effect of different grain size is investigated. Figure 6(a) and Figure 7 show all the interfaces that experience any level of damage, as stated in Eq. (39), but a deeper analysis of results shows that when the damage evolution is divided in three stages (i.e. \(0 < d \leq 0.5\), \(0.5 < d < 1\) and \(d = 1\)) all the three microstructures exhibit damage in the range \(0 < d \leq 0.5\); the only exception is the coarse grain structure which shows higher levels of damage. This behaviour is in good agreement with physical and literature results \[1\] and can be motivated as follows: in a fine grain structure the number of interfaces absorbing the load is higher and this mitigates the load on each interface; in other words in coarse grain microstructures the density of load per interface is higher than in finer grain aggregates. This could be also the reason for which the same level of damage in the early stage of the simulations is experienced at lower loads in coarse grains (insert in Figure 6(a)): the distribution of the same load on a smaller number of interfaces leads to higher stress concentration that is dissipated through damage onset.

On the other hand the behaviour at high \(\Delta \theta\), where \(\rho_c\) is larger for smaller grain size, can be explained as follows: since the region of stress relief upon damage onset or crack formation scales as \(a^2\) (\(a\) being the length of crack), the higher \(\rho_c\) at small \(\Delta \theta\) for coarse grain size is equivalent to the formation of longer cracks, which hence relieve stresses on a larger surface, preventing in this way the growth of additional damage. In other words, according to \[8\], \(\rho_c \propto 1/\bar{d}_{gr}\).
Another aspect on which attention has to be drawn is the extent of damage. The values of $\rho_c$ here suggest that 50% or 60% of the total interfaces experience at least some damage. However this also suggests the absence of a recognisable main pattern of the damage which instead is spread across the microstructure; this happens clearly due to the unconstrained thermal loading.

It is worth noting that if the degradation parameter $D$ was calculated for this case, the net tensile stress calculated with Eq. (40) during the unconstrained simulations would be equal to zero (due to the absence of any external constrain); an alternative way of retrieving the overall level of damage of the microstructure could be applying a strain load in post-processing and calculate the net tensile stress. With the presence of cohesive damage however the response of the aggregate would not be linear, and the stress calculated would depend on the strain applied. Since for these simulations the level of damage at the interfaces is not high, it is reasonable to assume that the non-linearity effect is not dominant and hence a reference strain can be applied to the three microstructures at different stages of the damage propagation in order to evaluate the average stresses and apply Eq. (45) to obtain the degradation $D$. Hence Figure 6(b) shows the damage $D$ as a function of the thermal loading for the three unconstrained microstructures.

Figure 8 shows instead the damaged interfaces in the three aggregates when tough grain boundaries have been considered ($R = 1$), and then either inter- and trans- granular damage is present in the microstructures. As it can be noticed, the number of transgranular surfaces decreases as the grain size decreases; moreover the transgranular damage is not developed through the whole length of the grain in the majority of the cases, but just onset from the grains’ boundaries occurs. This happens again because of the presence of a local mechanism responsible of damage onset and the lack of a mechanism driving the damage through the
Figure 7: Damaged interfaces in constrained microstructures with different grains’ size and weak grain boundaries ($R = 0.7$).

Figure 8: Damaged interfaces in constrained microstructures with different grains’ size and tough grain boundaries ($R = 1$).

structure. Curves showing $\rho_c$ and $D$ for the case of tough grains are not shown here for the sake of conciseness, because the additional transgranular damage, does not add any significant difference to the fraction of damaged interfaces and the residual strength.

When an $Al_2O_3$ grain is in contact with a $SiC$ grain and they both experience the same cooling ($\Delta \theta < 0$), the former will be tense and the latter will be compressed, simply because of the differential thermal strains (see Table 1). As mentioned in the Section 4 this behaviour was investigated in [3], where the stresses in two grains in contact due to thermal expansion
mismatch were expressed as:

\[ \sigma_{1}^{TEA} = -\sigma_{2}^{TEA} = \frac{1}{2} \Delta \alpha E (T_{sf} - T) \]  

(46)

where \( \Delta \alpha \) is the difference between the two coefficients of thermal expansion, \( E \) is the Young’s modulus, \( T_{sf} \) the temperature at which the microstructure is stress-free and \( T \) is the current temperature. Figure 9 shows the local variation of the stresses in a contour plot for a 50 grains microstructure; the values of stresses are in very good agreement with Eq. (46).

4.1.2. Constrained micro-structures

In the following simulations damage and micro-cracking propagation have been investigated in microstructures that have been rigidly constrained as if held between the grips of a testing machine. If for the unconstrained simulations the only mechanism able to lead to damage is the effect of the local thermal contraction mismatch, when instead the edges of the aggregates are constrained and a quasi-static thermal load is applied, the mechanical strain is different from zero and equal and opposite to the overall thermal strain (\( \varepsilon_{mech} = -\varepsilon_{\theta} \)), which consequently causes a net tensile stress different from zero that is conceptually very similar to the effect of mechanical loading. This overall stress is superimposed to the local effect of differential thermal expansion; however as it will be shown the net tensile stress is predominant and it is the mechanism driving damage propagation. For the sake of conciseness and since it
is believed that phenomenologically here the damage development depends strongly on the interaction between intergranular and transgranular microcracking, in this section only the case of tough grain boundaries has been considered \((R = 1)\).

Figure 10 shows the evolution of damage in the three microstructures considered in Figure 5, where the left and right edges have been fully constrained while top and bottom edges have been considered traction free; increasing uniform cooling thermal load \((\Delta \theta < 0)\) has been applied across the microstructures. It is interesting to notice that by comparing the three cracking developments, the coarse grain morphologies are more prone to experience transgranular damage than finer ones; this behaviour results in smoother crack paths as the grain size increases, in good agreement with [1].

As in Section 4.1.1 also in this case the cumulative damage length has been plotted: results are shown in Figure 11(a). A comparison between these curves and those in Figure 6(a) shows a few interesting differences: (i) for the unconstrained microstructure the temperature range is higher as it was expected, since in fact the presence of constraints reduces drastically the thermal load required to initiate damage; (ii) the curves for constrained case reach a sort of saturation that is not present in the unconstrained simulations; this saturation in \(\rho_c\) is attributable to the development of a main crack whose length is comparable to the size of the microstructure. Moreover Figure 11(a) shows that at high \(\Delta \theta\) the curve relative to the finer aggregate \((G = 13.5)\) falls between the other two; hence if the problem was studied focusing purely on the damage of the interfaces and independently from the level of degradation, those curves would suggest that excessive grain refinement could be detrimental for the microstructure and then an optimum grain size would be required; this behaviour depends of course on the delicate interaction and competition between the inter- and transgranular modes of fracture, whose balance gives the overall microscopic behaviour of the polycrystalline aggregate.

However studying the problem only in terms of damaged interfaces would be restrictive, so in the framework of multi-scale applications where the properties at the macroscale are retrieved through the features at the microscale, the degradation parameter \(D\) introduced in Eq. (45) has been used here to obtain more information on the residual strength of the three microstructures. From Figure 11(b) it is easy to notice that the degradation of the microstructure is faster as the grain size decreases. This behaviour is in good agreement with the case of mechanical loading where, generally speaking, coarse grain structures show a more brittle behaviour than finer grains.

Finally a clarification is due here. When comparing Figure 11(a) to the results obtained in [3], it is easy to notice that all the curves exhibit a plateau, which is related to the aforementioned saturation behaviour. However in the present work, the saturation of \(\rho_c\) is equivalent to the complete failure of the microstructure, as it is evident from Figure 10; the same is not true for simulations in [3], where instead the thermal load was further
\[ \Delta \theta = -175^\circ C \]

\[ G = 11.7 \]

\[ G = 12.5 \]

\[ G = 13.5 \]

\[ \Delta \theta = -300^\circ C \]

Figure 10: Inter-granular and Trans-granular damage evolution for different sizes of grains \( G \) and \( R = 1 \).
increased after saturation, with corresponding further rise of $\rho_c$ at higher $\Delta \theta$. Hence if for the constrained microstructure one compares the range where the curves show a plateau it results evident how the difference among the curves is not as significant as the case for unconstrained microstructures.

4.2. Transient

In this section numerical simulations using the transient model will be presented. Before dealing with polycrystalline microstructures, some examples are shown and comparisons with results obtained through finite element method are presented in order to validate the formulation.

Figure 12(a) shows a square plate with an adiabatic central crack, where the bottom, right and top edges are thermal insulated ($q = 0$) and a cooling linear thermal load ($\Delta \theta(t)$) is applied at the left edge (Figure 12(b)). Figure 13(a) and Figure 14(a) show the contour plots of the internal stresses $\sigma_{xx}$ at two time steps (0.4 sec and 3.5 sec.); Figure 13(b) and Figure 14(b) show instead the stress values $\sigma_{xx}$ along the line indicated by the dots in Figure 12(a), at the aforementioned time steps, as a comparison with the results obtained with a finite element commercial software: it is evident that the results are in very good agreement.

**Transient in microstructures**

In this section the effect of transient thermal loading on polycrystalline microstructures will be investigated. So far quasi-static thermal loading has been applied to the microstructures, and it has been shown that even without any external constrain, damage onset is possible due to differential thermal expansion between different phases. However it is well known
Figure 12: Plate with crack: (a) plate with loading and boundary conditions; (b) thermal loading \( \Delta \theta(t) \) applied at left edge \( (x = 0) \).

Figure 13: Stresses in cooled plate with crack at 0.4 sec.: (a) contour plot; (b) comparison between FEM and BEM stress profiles along horizontal central line.

that some polycrystalline ceramics have excellent thermal shock resistance, hence it is for this reason that a transient formulation is required when thermal loadings are applied very fast (i.e. shocks) and then a sequence of equilibrium statuses cannot be assumed. In this context it is useful to introduce the thermal shock resistance as a parameter to establish the
maximum temperature jump sustainable by the structure \[34\]:

\[
\Delta\theta_{\text{shock}} = A \frac{\sigma_f}{E \alpha} \frac{1}{Bi} = \frac{A \sigma_f k}{E \alpha \ h l}
\]  

(47)

where \(Bi\) is the Biot number, which gives an adimensional index of the ratio between heat transfer at the surface of the structure and inside it, \(h\) is the convective heat transfer coefficient, \(l\) is a characteristic dimension, \(k\) is the thermal conductivity; \(A\) is a parameter dependent on cold or hot shock and \(\sigma_f\) is the tensile strength (that here can be assumed as the maximum cohesive strength \(T_{max}\)). \(Bi = \infty\) is for perfect heat transfer and \(Bi \ll 1\) is for cases where the internal conduction is very fast and hence the interior of the structure can be assumed always at the same temperature (even with thermal flux passing through the body). The explicit presence of the Biot number in Eq. (47) is useful to assess the behaviour of materials during thermal processes such as quenching in different surrounding media (i.e. air or oil). However in the present model the convective heat transfer with the surrounding media has not been modelled and since all the microstructures compared here have the same dimension, the thermal resistance could be normalized by \(hl\) and re-defined as:

\[
R_{\text{shock}} = A \frac{k \sigma_f}{E \alpha} 
\]  

(48)

Values of \(R_{\text{shock}}\) for the two materials are: \(R_{\text{shock}}^{\text{SiC}} = 31.9\) and \(R_{\text{shock}}^{\text{Al2O3}} = 2.5\).

(a)

(b)

**Figure 14:** Stresses in cooled plate with crack at 3.5 sec.: (a) contour plot; (b) comparison between FEM and BEM stress profiles along horizontal central line.
Figure 15: Temperature variation with time at microstructure’s core for SiC, Al₂O₃ and 50% multiphase.

Another material property that affects the behaviour of the structure in presence of thermal shock is the thermal diffusivity; this property is the one responsible for the rapidity with which the steady state is reached in a structure and it is evident from Table 1 that SiC and Al₂O₃ have very different values of $\kappa$.

Figure 15 shows the temperature variation with time at the core of three 50-grains microstructures when a cooling thermal shock $\Delta \theta = -1000^\circ C$ is applied at the outer boundary; the three microstructures considered are SiC, Al₂O₃ and a multiphase of the previous two with volume ratio of 50%. It is clear comparing the three curves that the convergence to thermal uniformity in the multi-phase aggregate is influenced by the high diffusivity of silicon carbide.

Furthermore, as it has been said before, an index of the resistance to thermal shock could be the maximum temperature jump that a structure can bear without any damage or conversely as the damage extent due to a given temperature jump.

When interfaces damage (left legend) and internal stresses (right legend) are compared, as in Figure 16(a) and (b) it is interesting to note that for the single phase microstructures the stress develops purely because of the thermal gradient between outside and inside; Al₂O₃ shows higher damage intensity, coherently with what expected. Moreover the damage onset is “radial” coherently with the temperature propagation, and mainly localised at the external edges, as shown in Figure 16(c) and (d). In both cases the microstructures reach a stress-free status upon steady-state temperature distribution, since no external constraints have been applied.

On the other hand when damage and stresses are analysed in the multi-phase microstructure, transient thermal gradients and thermal expansion mismatch are two concurrent mechanisms of stress generation and damage onset. Figure 17 shows the early stage temperature
Figure 16: Interface damage levels and internal stresses (a, b) and damage pattern (c, d) in silicon carbide and aluminium oxide microstructures due to cooling thermal shock $\Delta \theta = -1000^\circ C$. Figures are taken at the time step where stresses are highest and damage already fully developed, corresponding to a core temperature $\Delta \theta_{\text{core}} = -80^\circ C$.

Propagation ($\Delta \theta_{\text{core}} = -56^\circ C$) in the multi-phase aggregate, the corresponding stress distribution and damage location; it is easy to notice that in this first stage the damaged interfaces are circumscribed to the area affected by the high thermal gradient between outside and inside and the "radial" pattern is present again.

However upon steady-state temperature distribution (uniform) the thermal expansion mismatch remains present, causing tense and compressed zones inside the aggregate (as shown in Figure 18(b)) instead of stress-free status; consequently this causes damage to be spread across the whole microstructure. Moreover the intensity of damage is less severe than pure $Al_2O_3$ (Figure 18(b)). Summarizing it is possible to conclude that due to the high
thermal shock resistance of silicon carbide, the multiphase aggregate behaves better than alumina; however due to difference in thermal expansion coefficients between the two phases, an additional feature must be taken into account, i.e. the possibility to have low level but spread damage throughout the microstructure.

**Figure 17:** Temperature (a) and stress (b) distributions in multi-phase microstructure after $\tau = 1 \times 10^{-6}$ sec from thermal shock. Damaged interfaces highlighted in red.

For the sake of completeness a comparative plot is shown in Figure 19. This curves help in understanding the effect of a thermal shock on a single-phase and multi-phase microstructure. It is worth noting that in this case, as well as the unconstrained examples shown before
in Section 4.1.1, the external boundary is traction free, so the application of the averaging theorem for the evaluation of the homogenised stress would give a damage parameter $D$ equal to zero. However overall strains can be evaluated thanks to Eq. (42).

It is evident from Figure 19 that the damage propagation mechanism in single-phase and multi-phase microstructures is different: in the former the propagation and hence increase in $\rho_c$ is related purely to the thermal gradient across the aggregate, so as the thermal gradient mitigates, the propagation arrests itself (shown by the curve relative to SiC and Al$_2$O$_3$) while thermal strain keeps increasing until uniform temperature distribution is reached; in the latter instead the initial mechanism is driven by the high thermal gradient but even when this mitigates, the local thermal expansion mismatch cause the damage to further propagate across the aggregate, due to the residual stresses stored in the grains and dissipated through cohesive damage.

5. Conclusion

In this paper the effect of thermo-mechanical loading has been studied in polycrystalline microstructures with different material properties, with the boundary element method. The model is able to take into account intergranular and transgranular damage evolution with a cohesive approach, which affects not only the mechanical properties of the interface but also its thermal conductivity; upon failure non-linear frictional contact analysis is introduced and micro-cracks are considered adiabatic ($q = 0$). Results have been presented for single-phase materials as well as for multi-phase aggregates and the features of stress development, damage

![Figure 19: Variation of strain $\varepsilon_{xx}$ with length of damage $\rho_c$.](image-url)
onset and propagation have been highlighted for steady-state and transient thermal loading. It is clear from the results that the presence of additional phases to a material could enhance some features of the overall structure but also new mechanisms of failure could develop, such as thermal expansion mismatch. Hence the improvement of thermo-mechanical behaviour of microstructures through the use of ceramic composites has to be the result of a tuning operation, where the development of the aggregate is tailored to the required application. The cohesive formulation used in this paper has given an interesting insight on the damage evolution: depending on the material properties, constraining and loading condition, not only can the damage propagation be localized in some specific zones of the microstructure or spread throughout it, but also the severity of debonding could be significantly affected. Bearing in mind that thermal processes are commonly done at the beginning of the operational life of the structural component, all these different behaviours affect its residual life and hence understanding the microscopic behaviour of polycrystalline materials become key in order to be able to predict the behaviour of macroscopic components.

A. Fundamental solutions

Defining the distance $r$ between collocation ($x'$) and integration ($x$) point as:

$$ r = \sqrt{(x_1 - x'_1)^2 + (x_2 - x'_2)^2} $$

(A.1)

and

$$ \frac{\partial r}{\partial n} = r_k n_k ; \quad k = 1, 2 $$

(A.2)

where Einstein notation has been used, the fundamental solutions used in the equations involved in the presented formulations are shown in the following section.

A.1. Steady-state

Displacement equation

$$ U_{ij}(x', x) = \frac{1}{8\pi\mu(1 - \nu)} \left\{ (3 - 4\nu) \log \left( \frac{1}{r} \right) \delta_{ij} + r_{,i}r_{,j} \right\} $$

(A.3)

$$ T_{ij}(x', x) = \frac{-1}{4\pi(1 - \nu)r} \left\{ \frac{\partial r}{\partial n} \left[ (1 - 2\nu)\delta_{ij} + 2r_{,i}r_{,j} \right] - (1 - 2\nu)(r_{,i}n_j - r_{,j}n_i) \right\} $$

(A.4)
\[
P_i(x',x) = \frac{(1+\nu)\alpha}{4\pi(1-\nu)} \left\{ \left[ \log \left( \frac{1}{r} \right) - \frac{1}{2} \right] n_i - r_i r_k n_k \right\}
\]  
(A.5)

\[
Q_i(x',x) = -\frac{(1+\nu)\alpha}{4\pi k(1-\nu)} \alpha r_{r,i} \left[ \log \left( \frac{1}{r} \right) - \frac{1}{2} \right]
\]  
(A.6)

**Traction equation**

\[
D_{ij}(x',x) = \frac{1}{4\pi(1-\nu)} \left\{ (1-2\nu)(-r_i r_j \delta_{ij} + r_j \delta_{ki} + r_i \delta_{jk}) + 2r_i r_j r_k \right\}
\]  
(A.7)

\[
S_{ij}(x',x) = \frac{\mu}{2\pi(1-\nu)} \frac{1}{r^2} \left\{ 2 \frac{\partial r}{\partial n} [(1-2\nu) r_i \delta_{ij} + \nu (r_j \delta_{ki} + r_i \delta_{jk}) - 4r_i r_j r_k] + 2\nu (n_i r_j r_k + n_j r_i r_k) + (1-2\nu) (2n_k r_i r_j + n_j \delta_{ki} + n_i \delta_{jk}) + -(1-4\nu) n_k \delta_{ij} \right\}
\]  
(A.8)

\[
P_{ij}(x',x) = \frac{\mu(1+\nu)\alpha}{2\pi(1-\nu)} \left\{ r_k n_k \left[ \frac{\delta_{ij}}{(1-2\nu)} - 2r_i r_j \right] + n_i r_j + n_j r_i \right\}
\]  
(A.9)

\[
Q_{ij}(x',x) = -\frac{\mu(1+\nu)\alpha}{2\pi k(1-\nu)} \left\{ r_j r_{r,j} + \frac{\delta_{ij}}{(1-2\nu)} \left[ \frac{(1+2\nu)}{2} - \log \left( \frac{1}{r} \right) \right] \right\}
\]  
(A.10)

**Temperature equation**

\[
\theta^*(x',x) = \frac{1}{2\pi k} \log \frac{1}{r}
\]  
(A.11)

\[
q^*(x',x) = \frac{r_i n_i}{2\pi r}
\]  
(A.12)
Flux equation

\[ \theta^*_i(x', x) = \frac{r^*_i(x', x)}{2\pi r} \] (A.13)

\[ q^*_i(x', x) = k \left( \frac{r^*_i x' n_i}{\pi r^2} - \frac{n_i}{2\pi r^2} \right) \] (A.14)

A.2. Transient

In this section the fundamental solutions resulting from the analytical temporal integration are presented; according to what explained in Section 3.3.1, linear time interpolation has been used. In the following relationships the quantity \( s_f \) has been defined as:

\[ s_f = \frac{r^2}{4\kappa(\tau_F - \tau_f)} \] (A.15)

and the exponential integral

\[ E_1(s_f) = \int_{s_f}^{\infty} e^{-x} dx \] (A.16)

has been evaluated using the polynomial approximations defined in [43].

Displacement equation

\[ f_i = \frac{(1 + \nu)\alpha}{4\pi(1 - \nu)} \left\{ (2r_i x' n_k - n_i) \left[ \frac{(1 - e^{-s_f})}{s_f} + \frac{(1 - e^{-s_{f-1}})}{s_{f-1}} \right] + \frac{n_i}{2} \left[ E_1(s_f) - E_1(s_{f-1}) \right] \right\} \] (A.17)

\[ \int_{\tau_{f-1}}^{\tau_f} F_i M^b d\tau = \]

\[ = \left\{ -(F - f) f_i - \frac{(1 + \nu)\alpha r^2}{32\pi(1 - \nu)\kappa \Delta \tau} \left\{ (r_i x' n_k - n_i) \left[ \frac{(1 - e^{-s_f})}{s_f^2} - \frac{(1 - e^{-s_{f-1}})}{s_{f-1}^2} \right] \right\} + \right. \]

\[ + (r_i x' n_k + \frac{n_i}{2}) \left[ E_1(s_f) - E_1(s_{f-1}) \right] - \left( \frac{e^{-s_f}}{s_f} - \frac{e^{-s_{f-1}}}{s_{f-1}} \right) \}

\[ + (F - f + 1) f_i + \frac{(1 + \nu)\alpha r^2}{32\pi(1 - \nu)\kappa \Delta \tau} \left\{ (r_i x' n_k - n_i) \left[ \frac{(1 - e^{-s_f})}{s_f^2} - \frac{(1 - e^{-s_{f-1}})}{s_{f-1}^2} \right] \right\} + \]

\[ + (r_i x' n_k + \frac{n_i}{2}) \left[ E_1(s_f) - E_1(s_{f-1}) \right] - \left( \frac{e^{-s_f}}{s_f} - \frac{e^{-s_{f-1}}}{s_{f-1}} \right) \} \]
\[ g_i = \frac{(1 + \nu)\alpha r_i}{4\pi k(1 - \nu)} \left\{ \left[ -\frac{(1 - e^{-s_f})}{s_f} + \frac{(1 - e^{-s_{f-1}})}{s_{f-1}} \right] - \frac{1}{2} \left\{ E_1(s_f) - E_1(s_{f-1}) \right\} \right\} \]  
\[ (A.18) \]

\[ \int_{\tau_{j-1}}^{\tau_j} G_i M^k d\tau = \left[ -(F - f)g_i - \frac{(1 + \nu)\alpha r_i}{64\pi k(1 - \nu)\kappa \Delta \tau} \left\{ \left[ \frac{(1 - e^{-s_f})}{s_f^2} - \frac{(1 - e^{-s_{f-1}})}{s_{f-1}^2} \right] + \right\} \right. \\
\left. + \left( \frac{e^{-s_f}}{s_f} - \frac{e^{-s_{f-1}}}{s_{f-1}} \right) - \left[ E_1(s_f) - E_1(s_{f-1}) \right] \right\} \]  
\[ (A.19) \]

\[ (F - f + 1)g_i + \frac{(1 + \nu)\alpha r_i}{64\pi k(1 - \nu)\kappa \Delta \tau} \left\{ \left[ \frac{(1 - e^{-s_f})}{s_f^2} - \frac{(1 - e^{-s_{f-1}})}{s_{f-1}^2} \right] + \right\} \]
\[ \left. + \left( \frac{e^{-s_f}}{s_f} - \frac{e^{-s_{f-1}}}{s_{f-1}} \right) - \left[ E_1(s_f) - E_1(s_{f-1}) \right] \right\} \]  
\[ (A.20) \]

**Traction equation**

\[ f_{ij} = \frac{E\alpha}{4\pi(1 - \nu)r} \left\{ r_{,j}n_i + r_{,i}n_j + r_{,m}(\delta_{ij} - 4r_{,i}r_{,j}) \right\} \left[ \frac{(1 - e^{-s_f})}{s_f} - \frac{(1 - e^{-s_{f-1}})}{s_{f-1}} \right] + \]
\[ 2r_{,m}(r_{,i}r_{,j} + \frac{\nu \delta_{ij}}{1 - 2\nu})(e^{-s_f} - e^{-s_{f-1}}) \]  
\[ (A.21) \]
\[
\int_{r_{f-1}}^{r_f} F_{ij} M^b d\tau = \left\{-\left(F - f\right)f_{ij} - \frac{E\alpha r}{32\pi(1 - \nu)\kappa\Delta \tau} \left\{ (4r_i r_j r_i r_j - r_j n_i - r_i n_j - \delta_{ij} r_i n_i) \\
- \left(\frac{1 - e^{-s_f}}{s_f^2} - (1 - e^{-s_{f-1}})\right) - \left(\frac{e^{-s_f}}{s_f} - \frac{e^{-s_{f-1}}}{s_{f-1}}\right)\right\} \right\} \\
- \left(r_j n_i + r_i n_j + \delta_{ij} \frac{(1 + 2\nu)}{(1 - 2\nu)} r_i n_i\right) \left[E_1(s_f) - E_1(s_{f-1})\right]\left(E_1(s_f) - E_1(s_{f-1})\right)\right\} \right\} \\
= \left\{(F - f + 1)f_{ij} + \frac{E\alpha r}{32\pi(1 - \nu)\kappa\Delta \tau} \left\{ (4r_i r_j r_i r_j - r_j n_i - r_i n_j - \delta_{ij} r_i n_i) \\
- \left(\frac{1 - e^{-s_f}}{s_f^2} - (1 - e^{-s_{f-1}})\right) - \left(\frac{e^{-s_f}}{s_f} - \frac{e^{-s_{f-1}}}{s_{f-1}}\right)\right\} \right\} \\
- \left(r_j n_i + r_i n_j + \delta_{ij} \frac{(1 + 2\nu)}{(1 - 2\nu)} r_i n_i\right) \left[E_1(s_f) - E_1(s_{f-1})\right] \left(\frac{(1 + 2\nu)}{(1 - 2\nu)} r_i n_i\right) \left[E_1(s_f) - E_1(s_{f-1})\right] \right\} \\
- \left(\frac{\delta_{ij}}{2} \frac{(1 + 2\nu)}{(1 - 2\nu)} \right) \left[E_1(s_f) - E_1(s_{f-1})\right] \left[E_1(s_f) - E_1(s_{f-1})\right] \right\} (A.22)
\]

\[
g_{ij} = \frac{E\alpha}{4\pi k(1 - \nu)} \left\{ \left(\frac{\delta_{ij}}{2} - r_i r_j\right) \left(\frac{1 - e^{-s_f}}{s_f} - (1 - e^{-s_{f-1}})\right) + \right. \\
\left. \frac{\delta_{ij}}{2(1 - 2\nu)} \left[E_1(s_f) - E_1(s_{f-1})\right]\right\} (A.23)
\]

\[
\int_{r_{f-1}}^{r_f} G_{ij} M^b d\tau = \left\{-\left(F - f\right)g_{ij} - \frac{E\alpha r^2}{32\pi k(1 - \nu)\kappa\Delta \tau} \left\{ (r_i r_j - \frac{\delta_{ij}}{2}) \left(\frac{1 - e^{-s_f}}{s_f^2} - (1 - e^{-s_{f-1}})\right)\right\} \right\} \\
- \left(\frac{\delta_{ij}}{2} \frac{(1 + 2\nu)}{(1 - 2\nu)} \right) \left[E_1(s_f) - E_1(s_{f-1})\right] \left[E_1(s_f) - E_1(s_{f-1})\right] \right\} \right\} \\
= \left\{(F - f + 1)g_{ij} + \frac{E\alpha r^2}{32\pi k(1 - \nu)\kappa\Delta \tau} \left\{ (r_i r_j - \frac{\delta_{ij}}{2}) \left(\frac{1 - e^{-s_f}}{s_f^2} - (1 - e^{-s_{f-1}})\right)\right\} \right\} \\
- \left(\frac{\delta_{ij}}{2} \frac{(1 + 2\nu)}{(1 - 2\nu)} \right) \left[E_1(s_f) - E_1(s_{f-1})\right] \left[E_1(s_f) - E_1(s_{f-1})\right] \right\} \right\} (A.24)
\]
Temperature equation

\[ \Theta^f = -\frac{1}{4\pi k} [E_1(s_f) - E_1(s_{f-1})] \]  
(A.25)

\[ \int_{\tau_{f-1}}^{\tau_f} \Theta^* M^b d\tau = \left[ -(F - f)\Theta^f - \frac{r^2}{16\pi k \Delta \tau} \left\{ \left[ \frac{e^{-s_f}}{s_f} - \frac{e^{-s_{f-1}}}{s_{f-1}} \right] \right\} 
- \left[ E_1(s_f) - E_1(s_{f-1}) \right] \right] 
- \left[ E_1(s_f) - E_1(s_{f-1}) \right] \]  
(A.26)

\[ Q^f = -\frac{r_i n_k}{2\pi r} [e^{-s_f} - e^{-s_{f-1}}] \]  
(A.27)

\[ \int_{\tau_{f-1}}^{\tau_f} Q^* M^b d\tau = \left[ -(F - f)Q^f - \frac{r_i n_k r^2}{8\pi k \Delta \tau} \left[ E_1(s_f) - E_1(s_{f-1}) \right] \right] 
+ \left[ (F - f + 1)Q^f + \frac{r_i n_k r^2}{8\pi k \Delta \tau} \left[ E_1(s_f) - E_1(s_{f-1}) \right] \right] \]  
(A.28)

Flux equation

\[ \Theta^i = -\frac{r_i}{2\pi r} \left[ -e^{-s_f} + e^{-s_{f-1}} \right] \]  
(A.29)

\[ \int_{\tau_{f-1}}^{\tau_f} \Theta_i^* M^b d\tau = \left[ -(F - f)\Theta^i - \frac{r_i r_{i,t}}{8\pi k \Delta \tau} \left[ E_1(s_f) - E_1(s_{f-1}) \right] \right] 
- \left[ E_1(s_f) - E_1(s_{f-1}) \right] \]  
(A.30)

\[ Q_i^f = \frac{k}{\pi r^2} \left( \frac{n_i}{2} - r_i n_k r_{i,t} \right) (e^{-s_f} - e^{-s_{f-1}}) - \frac{c_s r_i n_k r_{i,t}}{4\pi} \left( \frac{e^{-s_f}}{(\tau_F - \tau_f)} - \frac{e^{-s_{f-1}}}{(\tau_F - \tau_{f-1})} \right) \]  
(A.31)
\[
\int_{\tau_{f-1}}^{\tau_f} Q_{f}^{**} M^{b} \, d\tau = \left[ - (F - f) Q_{f}^{f} + \frac{n_{x} c_{e}}{8\pi \Delta T} \left[ E_{1}(s_{f}) - E_{1}(s_{f-1}) \right] + \frac{c_{e} r_{k} n_{k} f_{,\delta}}{4\pi \Delta T} \left[ e^{-s_{f}} - e^{-s_{f-1}} \right] \\
(F - f + 1) Q_{i}^{f} - \frac{n_{i} c_{e}}{8\pi \Delta T} \left[ E_{1}(s_{f}) - E_{1}(s_{f-1}) \right] + \frac{c_{e} r_{k} n_{k} f_{,\delta}}{4\pi \Delta T} \left[ e^{-s_{f}} - e^{-s_{f-1}} \right] \right]
\]

(A.32)

In the previous equations the two components of each integration resulting from linear time interpolation refer to the two temporal nodes of the generic time step \( f \), and the shape functions are written in Eq. [31].

B. Local fields

The integral boundary equations presented in the previous sections have been written in terms of the local component of the interfaces, in order to facilitate the application of interface conditions and the development of cohesive damage. Thus all the prescribed boundary conditions are enforced in the local coordinate system of each element:

\[
\tilde{t}^{p} = R \ t^{p} \quad ; \quad \tilde{u}^{p} = R \ u^{p}
\]

(B.1)

where \( t^{p} \) and \( u^{p} \) are the prescribed tractions and displacements and \( R \) is the transformation matrix to rotate from global coordinate to normal and tangential local coordinate, \( n_{x} \) and \( n_{y} \) being the components of the normal unit vector on the boundary \( S^{H} \):

\[
R = \begin{bmatrix}
-n_{y} & n_{x} \\
n_{x} & n_{y}
\end{bmatrix}
\]

(B.2)

The fundamental solutions need to be rotated too, in order for them to correspond to the unknown field in local (tangential-normal) coordinate:

\[
\tilde{T} = T \ R \quad ; \quad \tilde{U} = U \ R
\]

(B.3)

From a modelling point of view in the more general case of orthotropic material, the equations are written in material coordinate so that the rotation of the fourth order compliance tensor is avoided and hence each grain coordinate expressed by \( x_{S^{H}} \in S^{H} : x_{S^{H}} \subset \mathbb{R}^{2} \) is rotated to the material coordinate system \( \tilde{x}_{S^{H}} \in \tilde{S}^{H} : \tilde{x}_{S^{H}} \subset \mathbb{R}^{2} \). Each grain is then rigidly rotated by the angle \( \theta \):

\[
\dot{x}_{S^{H}} = R_{\theta} \ x_{S^{H}}
\]

(B.4)
where

$$R_\theta = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix}$$ (B.5)

and a new rotation matrix has to be defined for the rotation of the fundamental solutions (Eq. (B.3)):

$$\tilde{R} = \begin{bmatrix} -\tilde{n}_y & \tilde{n}_x \\ \tilde{n}_x & \tilde{n}_y \end{bmatrix}$$ (B.6)

where $\tilde{n}_x$ and $\tilde{n}_y$ are the components of the normal unit vector on the boundary $\tilde{S}^H$. 

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References


[38] L. Onsager, Reciprocal relations in irreversible processes. i., Physical review 37 (4) (1931) 405.


Table 1: Materials’ properties

<table>
<thead>
<tr>
<th>Property</th>
<th>SiC</th>
<th>Al₂O₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (ρ)</td>
<td>$3.1 \times 10^{-6}$ kg/mm³</td>
<td>$3.69 \times 10^{-6}$ kg/mm³</td>
</tr>
<tr>
<td>Young’s modulus (E)</td>
<td>470 GPa</td>
<td>431 GPa</td>
</tr>
<tr>
<td>Poisson’s ratio (ν)</td>
<td>0.15</td>
<td>0.29</td>
</tr>
<tr>
<td>Coeff. thermal exp. (α)</td>
<td>$4 \times 10^{-6}$ °C</td>
<td>$8.4 \times 10^{-6}$ °C</td>
</tr>
<tr>
<td>Conductivity (k)</td>
<td>$120 \times 10^{-3}$ W/(mm K)</td>
<td>$18 \times 10^{-3}$ W/(mm K)</td>
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<tr>
<td>Specific Heat (c)</td>
<td>750 J/(Kg K)</td>
<td>880 J/(Kg K)</td>
</tr>
<tr>
<td>Diffusivity (κ)</td>
<td>51.6 mm²/s</td>
<td>10.2 mm²/s</td>
</tr>
<tr>
<td>Fracture toughness (K_{IC})</td>
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<td>3 MPa√m</td>
</tr>
<tr>
<td>Friction coeff. (μ_f)</td>
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<td>0.2</td>
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