A numerical approach to the analysis of failure modes in anisotropic plates

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**Abstract**

This study is motivated by the attempt to characterize failure modes of silicon chips commonly used in electronic industries. Previous experimental investigations provided the failure probability of dies made of a single-crystal and produced a large variety of crack patterns, but were not able to elucidate the link between defect distributions and crack initiation and propagation. To get some insight in the fracture activation and propagation mechanisms, we resort to finite element analyses and adopt an explicit methodology for crack tracking, based on the self-adaptive insertion of cohesive elements into a coherent mesh of solid elements. Finite kinematics material models with anisotropic features for both bulk and cohesive surfaces are employed to describe the behavior of single-crystal silicon plates undergoing a particular bending test up to failure. The cohesive model adopted in the calculation is fully anisotropic and newly formulated to accomplish the present study. Numerical simulations considering different material properties were able to ascertain the effects of particular flaws on failure modes of brittle silicon plates.

**Keywords:** Cohesive model, Anisotropic fracture, Orthotropic material, Finite element method, Silicon dies

**1. Introduction**

The heart of every microelectronic compound, the integrated circuit, is commonly built on single-crystal silicon wafers that possess a high level of purity and perfection. Aside from the need to be single-crystalline in nature, they must also have a high degree of chemical purity, a high degree of crystalline perfection, and high structure uniformity.

The raw silicon to be used for this purpose is produced from silicon ingots which are sliced into thin wafers, i.e., they undergo grinding, sawing and polishing procedures and, subsequently, the integrated circuits are build onto the wafers. Although there exist many distinct fabrication processes, they all consist of a long series of etching and deposition steps until the circuit is completed. A certain impairment of the wafer, e.g., by scratching and trimming voids, cannot totally be avoided during this process.

Quality management and functional assurance require the prediction of the failure probability of the silicon dies. Due to their brittle nature the strength data of silicon dies are scattered and a probabilistic approach to failure is required. As a consequence of fabrication, silicon dies show different populations of flaws. Flaw variability, in turn, causes a broad distribution of strengths that under supercritical loads may lead to different failure modes, in general characterized by tortuous crack patterns.

From the material science point of view, silicon is a brittle material with a cubic symmetry, i.e., a lattice of diamond structure. Single crystal silicon has been studied extensively for its fracture characteristics, see [2,3,9,16,18,21,22,8,29] to name a few. It has two principal cleavage planes: \{111\} planes, usually the easy cleavage plane, and \{110\} planes; cleavage fracture...
# Nomenclature

- **C** - spatial bulk constitutive tensor
- **E** - Young’s modulus
- **F** - deformation gradient tensor
- **G** - shear modulus
- **K** - effective cohesive stiffness
- **L** - characteristic cohesive zone length
- **m** - Weibull coefficient
- **n** - spatial normal to the cohesive surface
- **N** - material normal to the cohesive surface
- **P** - Weibull’s statistic distribution
- **P** - first Piola-Kirchhoff stress tensor
- **q** - internal variable vector
- **t** - effective cohesive traction
- **T** - material traction vector
- **X** - material position vector
- **a** - ratio between the minimum shear strength and maximum shear strength
- **b** - ratio between the maximum shear strength and maximum shear strength
- **d** - effective opening displacement
- **D** - opening displacement vector
- **e** - ratio between the maximum shear strength and the maximum normal strength
- **ε** - small strain tensor
- **e** - logarithmic strain tensor
- **ν** - Poisson’s coefficient
- **σ** - generic stress measure
- **ϕ** - cohesive free energy density
- **q** - deformation mapping
- **a_x** - spatial basis vector on the cohesive surface
- **a_x^*** - dual spatial basis vector on the cohesive surface
- **A^t_j** - component of the material basis vector on the cohesive surface
- **A^t_j** - material basis vectors on the cohesive surface
- **A^t_j** - dual material basis vectors on the cohesive surface
- **C^t_i^j^h^k** - spatial component of the bulk constitutive tensor
- **d_i** - spatial component of the opening displacement derivative
- **D^t_i^j** - spatial component of the cohesive constitutive matrix
- **e_R^S** - Levi-Civita symbol
- **E_i** - orthonormal basis vector
- **G^c_i** - material critical energy release rate in the direction i
- **I_i** - local principal basis vectors on the cohesive surface
- **K^c_i^t_j** - material cohesive stiffness components
- **m^t_x** - spatial dual principal axis of anisotropy on the cohesive surface
- **m_x** - spatial principal axis of anisotropy on the cohesive surface
- **m^t_x** - dual spatial principal axis of anisotropy on the cohesive surface
- **M_i** - material principal axis of anisotropy on the cohesive surface
- **N_a** - shape function for node a
- **N_{a,t_j}** - shape function derivative for node a
- **R^t_x** - derivative of the spatial basis vector on the cohesive surface
- **R_{a,t_j}** - derivative of the spatial normal on the cohesive surface
- **R^t_i** - rotation tensor from the principal anisotropy system to the cohesive surface
- **R^t_i** - rotation tensor on the cohesive surface
- **T_c** - cohesive resistance in the generic direction
- **T_{c_i}** - material cohesive resistance in the direction i
- **T_{c,M_1}** - maximum normal strength on the cohesive surface
- **T_{c,M_2}** - minimum normal strength on the cohesive surface
- **T_i** - material components of the cohesive traction vector
- **u_i** - displacement component
- **U_{a,t_j}** - displacement components of node a
- **x_i** - spatial position component
- **X_i** - material position component
ized and conducted experimentally as well as by finite element analysis, e.g., drop tests of packages [1,14,15,37] and simple bending tests [7,17]. Then, the sole information available to the analyst is the statistical distribution of the strength of the packages. More illuminating are, of course, reliability tests of single silicon wafers and dies, cf. [13,5,6]. In the particular case considered here, we refer to an experimental program on small silicon structures, performed to obtain the failure loads and to estimate life expectation and failure probability of silicon dies.

The first sets of experiments were based on standard three-point and four-point-bending tests. Regrettably, these traditional tests produced a large variety of fragmentation patterns and failure loads and lead to a combination of different damaging effects. They were not able to clarify the failure mechanisms and to correlate the presence and the density of material defects to the development of a specific mode of failure. In particular, some specimens of the same batch fail at very low loads, while others withstand very high loads. High quality materials should not present such a high variability in strength. Indeed, good products are characterized by a narrow strength distribution, whereas a broad distribution denotes a less advanced material, or, more likely here, it may indicate processing faults. For a better understanding of the mechanisms of failure, an alternative fracture test – the ball-on-edge test – was adopted and another set of experiments has been performed. Here it was possible to distinguish two different failure mechanisms and two different strength distributions. Unfortunately, the experiments were still not able to elucidate the development of the failure mechanisms.

The need to understand the mechanisms of die failure suggested to use the finite element method with fracturing features to simulate the experiments. The aim of this paper is to introduce a suitable theoretical and numerical approach for such finite element simulations. Clearly, a realistic numerical model of the die requires the characterization of the silicon material in the best way; therefore we consider an anisotropic elastic material model and account for finite kinematics. The actual onset and propagation of cracks is explicitly described by an adaptive fragmentation algorithm based on an anisotropic cohesive element technique. In general, the cohesive theory is well understood and accepted for analyzing failure of brittle materials under Mode I or mixed Mode loading. Fracture is described as the progressive separation of two surfaces across an extended crack tip (process zone), resisted by cohesive tractions. All the nonlinearities of the material, typically brittle and therefore unable to develop large plastic deformations, are accounted for by the cohesive law. Due to the presence of an intrinsic cohesive length scale, the process zone of a crack must be resolved suitably by the discretization. Consequently, the numerical fracture does not show spurious mesh dependency effects. Moreover, a finite element model permits to introduce controlled distributions of strength at precise locations in order to model flaws.

Although some theoretical spurious mesh dependency issues can be solved by using cohesive elements, it is important to observe that crack tracking in presence of branching is a very difficult task, and the choice of a discretization necessarily introduces mesh dependency. Notoriously, tackling crack branching requires special meshing algorithms, see, e.g., [27,28], and it is best achieved by adopting adaptive insertion of cohesive surfaces [26]. The issue of mesh dependency of crack patterns is under deep investigation in the computational mechanics community. As matter of fact, in a recent paper [11] we tackled the problem of mesh dependency for anisotropic fracture. In that study, we considered very regular meshes and observed a nice convergence with the mesh size.

It is clear that the efficiency of the approach proposed in this work should be assessed though a study of convergence upon refinement. Anyhow, we would like to stress the fact that aim of the present work is not to assess the quantitative performance of the model, but to define a methodology to include anisotropy in a cohesive model, and to explore the possibility to use it for the characterization of failure modes for a particular test of silicon dies.
It is worth to spend a few words about the choice of a continuum model instead of a reduced structural model, such as plate or shell. Actually, the thin structures under consideration may be modeled as plates. In the dimensional reduction of a given continuum to a quasi two-dimensional structure, characterized by a small thickness, the out-of-plane stress components are typically neglected. In this case, it is customary to assume a linearized model. Such an approach is justified when the problem is characterized by small displacements and strains, and it leads directly to the classical theories of Kirchhoff and Reissner-Mindlin, based on the assumptions of small strains and very small deflections. However, brittle fracture in silicon dies is usually preceded by a certain amount of deformation, in some cases small but often falling in the range of moderate deflections. Consequently, plate models based on a linearized kinematic do not cover all possible experimental setups and need to be replaced by more sophisticated theories such as von Karman or Wolmir [35]. Additionally, we are interested in considering material flaws located anywhere across the thickness, which cannot be easily described in a plate model. To avoid the complication and the limits of a complex structural model, we made recourse to the continuum theory.

The paper is organized as follows. In Section 2 we describe the experiments and provide some data obtained from the experimental program. Then, in Section 3, we describe the anisotropic material model used for the bulk. The material behavior is defined in terms of finite kinematics, and reduced to a linearized model through the logarithmic mapping. In Section 4, we introduce the anisotropic model for the cohesive surfaces. In Section 4.1 we start from the characterization of the resistance properties of the material, and derive the cohesive parameters to be used in the behavior of the interface created by a fracture propagation. In Section 4.2 we describe the kinematics of the cohesive surface, and in Section 4.3 the cohesive law and the derived tractions. The fully anisotropic cohesive model here adopted is new, has been developed for this work and has not been presented before. In Section 5 we illustrate several numerical simulations which underline the versatility of this approach. In particular, we consider global and local alteration of the material properties to evaluate the effects of imperfections on the failure modes.

2. Experimental setup and Weibull distribution

Typically, failure experiments on silicon dies are performed using simple geometries, e.g., three-point-bending tests, where the applied load is increased progressively until fracture occurs. Statistical strength parameters are determined from the experimental data. Regrettably, traditional bending tests are not able to ascertain the mean fracture stress in silicon, since specimens often fail with different failure mechanisms. Referring in particular to the experimental program above mentioned [4,5], several specimens failed at very low loads, denoting a flawed (or otherwise weakened) population. In general, most of the specimens showed an intermediate strength. By means of an alternative experimental setup, the Ball-on-Edge (BoE) test, it was possible to distinguish between two different failure modes, i.e., sets of cracks starting from the edge and from the surface of the die. This suggested the presence of two distinct sets of flaws, one at the edge — due to the cutting procedure — and one on the surface — due to the wafer processing.

Typically, the strength of a material is characterized by an S-shaped distribution. For brittle materials, such as silicon, the distribution of the fracture stress can be fitted reasonably well by a two-parameter Weibull distribution:

$$P(\sigma) = 1 - \exp \left[ - \left( \frac{\sigma}{\sigma_L} \right)^m \right]$$

Fig. 1. Loading configuration and geometry in mm of the Ball-on-Edge fracture test on silicon plates.
where $\sigma_L$ is a reference parameter, roughly equal to the strength at 63% of fracture probability, and $m$ is called Weibull coefficient. When a particular batch of specimens shows high variability in the fracture stress, the strength distribution is characterized by a small Weibull coefficient, while a low variability is related to a high Weibull coefficient.

The experimental setup of the BoE test is shown in Fig. 1; it is taken as reference in the present study. The plate is supported by three 2 mm diameter spheres, and the load is applied through a fourth sphere in proximity of the edge. A sample of 20 specimens was tested. All specimens were loaded up to fracture and the fracture loads were recorded, see Fig. 3 (left). However, the distribution of the fracture strength does not show the classic S-shape. This is mainly due to the two different failure modes; in particular, failure resulting from edge flaws is characterized by loads ($5 \cdot 10^3 \text{N}$) lower than the ones typically related to failure originated by surface flaws ($15 \cdot 20 \text{N}$). The fragments of the dies were preserved: typical fracture patterns, one related to surface failure, one related to edge failure, are shown in Fig. 2. The plates split in large fragments, except in the loading zone where, for surface failure, many small fragments are observed.

In the BoE experiments, it was possible to identify the Weibull parameters for the strength distribution of the plates. The edge mechanism was related to a strength distribution with $\sigma_L = 130 \text{ MPa}$ and $m = 2.8$; while the surface mechanisms was characterized by a narrower and stronger distribution, i.e. $\sigma_L = 295 \text{ MPa}$ and $m = 25.2$, see Fig. 3 (right). The Weibull parameters of the two failure modes suggest that the damage induced by the cutting in general is more invasive and localized, leading to a weaker and more dispersed resistance distribution; while the damage induced by the thinning procedure is uniformly distributed, less pernicious and easier to be controlled during the processing phase.

3. Bulk material

Silicon dies are characterized by a dependence on the direction of the elastic and resistance material properties. As a consequence of the cubic crystal lattice the material is stiffer in some directions and more compliant in other directions. Generally, the orthotropic behavior of a material is characterized by nine independent elastic coefficients in the elasticity tensor. In a linearized kinematic approach, the generalized Hooke’s law relates the Cauchy stress $\sigma$ and the linearized strain tensor $\varepsilon$ in the form:
\[ \sigma = C \varepsilon, \]

where the material tensor \( C \) has the components:

\[
\begin{bmatrix}
C_{1111} & C_{1122} & C_{1133} & 0 & 0 & 0 \\
C_{1122} & C_{2222} & C_{2233} & 0 & 0 & 0 \\
C_{1133} & C_{2233} & C_{3333} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{1212} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{1313} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{2323}
\end{bmatrix}.
\]

Here we made use of Voigt’s matrix notation, for readability. Silicon has cubic symmetry, i.e., it does not show the full orthotropic behavior described in (3). In particular, the stiffness in the \( \{100\} \)-crystal axes is, according to [36]:

- \( C_{1111} = C_{2222} = C_{3333} = 165.800 \text{ MPa} \)
- \( C_{1122} = C_{1133} = C_{2233} = 63.900 \text{ MPa} \)
- \( C_{1212} = C_{1313} = C_{2323} = 79.600 \text{ MPa} \)

The elastic constants are related to the engineering Young modulus \( E \), shear modulus \( G \) and Poisson’s coefficients \( \nu \) through the following relations:

\[
E = \frac{(C_{1111} - C_{1122})(C_{1111} + 2C_{1122})}{C_{1111} + C_{1122}}, \quad G = C_{1212}, \quad \nu = \frac{C_{1122}}{C_{1111} + C_{1122}}.
\]

Although we obtain in this way the same moduli in \( X_1, X_2 \) and \( X_3 \) direction, the material is not isotropic. The dependence of the elastic moduli on the direction is illustrated in Fig. 4. Here and in the following we assume our global coordinate system to be oriented in direction \( \{100\}, \{010\} \) and \( \{001\} \), respectively, i.e., the \( X_1-X_2 \) plane is the top surface of the die and \( X_3 \) is the out-of-plane axis. In Fig. 4, the symbol \( (\cdot) \) \( ^{\perp} \) denotes the value of the elastic constant in in-plane direction and the symbol \( (\cdot) \) \( ^{\parallel} \) denotes the elastic constant related to out-of-plane deformation.

As stated above, in our simulations we account for the full kinematics of finite deformation. We adopt the deformation gradient \( F \) as deformation measure and the first Piola-Kirchhoff stress tensor \( P \) as stress measure. The link between the small strain formulation and the finite kinematics formulation is achieved in a straightforward way by the use of exponential and logarithmic mappings. The logarithmic strain \( \varepsilon \) is defined through the deformation gradient \( F \) as:

\[
\varepsilon = \frac{1}{2} \log FF^T.
\]

Following [25] the calculation of the logarithmic strain is made in terms of spectral representation or Taylor’s expansion according to the magnitude of the strains. Strain tensor (4) is then employed in (2) to compute the Cauchy stresses \( \sigma \) and the 1st Piola-Kirchhoff stress tensor follows by:

\[
P = \det(F) \sigma F^{-T}.
\]

4. Fracture surfaces

Nucleation and propagation of cracks are efficiently modeled through the cohesive zone approach [3,10]. Within the framework of finite element discretization, cohesive theories lead directly to the interface element technique, here applied in the form introduced in [24]. The authors are aware of other approaches to compute crack propagation along a priori
unknown paths, such as embedded discontinuities or enriched elements. A comparison of the pros and cons of different numerical techniques, however, falls beyond the scope of this paper. Here we employ the classical cohesive element approach of [24], combined with the automatic fragmentation and cohesive surface insertion procedure described in [26]. The method has proven to be reliable and efficient for numerous applications, among them the analysis of dynamic crack propagation in unidirectional composites [38], anisotropic bulk material [31] and orthotropic fiber reinforced tissues [11,12]. In contrast to former works, where we assumed transverse isotropy [38], or orthotropy over the cohesive surface [11,12], here we construct the cohesive model without any restriction of material symmetry, since in finite kinematics also an initially orthotropic material may behave as fully anisotropic due to the change in orientation of the principal anisotropy axis. It follows that during the deformation the directions of distinct toughness and sliding properties may vary in an arbitrary way.

In cohesive theories, the opening displacements Δ across a cohesive surface S play the role of a deformation measure, while the tractions T furnish the work-conjugate stress measure. Supported by experimental evidence, the cohesive behavior, for both isotropic and anisotropic materials, is different for opening (Mode I separation) and sliding (Modes II and III separation). Additionally, an anisotropic cohesive model must be characterized by a law with cohesive properties (both strength and toughness) dependent on the direction of sliding on the cohesive surface.

The characterization of anisotropy along cohesive interfaces requires the definition of the planes of local material symmetry, of the local normal and shear fracture resistances and of the corresponding cohesive energies.

In the following, we assume a material point of view, and begin by establishing a relation between the cohesive parameters and the resistance of the bulk. The relation is based on the local orientation of the cohesive surface with respect to the principal anisotropy axes of the material in the reference configuration, see Section 4.1. Once the cohesive surface has been formed, its kinematics is defined by the relative motion of the confining subbodies through the displacement jump, see Section 4.2. Finally, following a thermodynamic approach, we define the traction work-conjugate to the displacement jump through a free energy density ϕ. Accordingly, we derive a fracturing criterion based on the cohesive traction measure, see Section 4.3.

4.1. Anisotropic cohesive parameters

Consider a generic point P of a body made of an orthotropic material. The principal anisotropy axes are identified by a set of orthonormal basis vectors. For the sake of simplicity, we assume that initially the anisotropy axes coincide with the reference axes of the body. While the anisotropy of the elastic stiffness is intrinsically built in the adopted elastic behavior, it is necessary to characterize the variation of the tensile resistance with the material direction. To this end we make use of a fracture resistance surface which bounds the effective cohesive properties, see Fig. 5. In the context of an initially orthotropic material an ellipsoidal resistance surface with principal axes in X1, X2 and X3 direction is the natural choice:

\[
\frac{X_1^2}{T_{c1}^2} + \frac{X_2^2}{T_{c2}^2} + \frac{X_3^2}{T_{c3}^2} - 1 = 0.
\]

Each principal material direction is characterized by a different tensile resistance, e.g., \(T_{c1} \geq T_{c2} \geq T_{c3}\). The corresponding critical energy release rates scale proportionally; then it follows \(G_{c1} \geq G_{c2} \geq G_{c3}\).

Under a finite element discretization of a solid body, the direction \(\mathbf{N}\) of interest identifies the normal to an inter-elemental surface in the reference configuration. During the evolutive analysis, the tractions acting on the surface will be compared to the local cohesive resistance within a fracture criterion. Assigned \(\mathbf{N}\), the cohesive resistance \(T_c(\mathbf{N})\) and the critical energy release rate \(G_c(\mathbf{N})\) are derived as follows. The straight line \(\mathbf{TN}\), with \(|\mathbf{N}| = 1\), is described through the coordinates \(X_j = T N_j\). Introducing the line coordinates in (5) and solving with respect the scalar \(T\), one obtains the sought critical resistance:

\[
T_c(\mathbf{N}) = \left[ \frac{N_1^2}{T_{c1}^2} + \frac{N_2^2}{T_{c2}^2} + \frac{N_3^2}{T_{c3}^2} \right]^{-1/2}.
\]

![Fig. 5. Fracture resistance surface.](image-url)
We assume that the critical energy release rate $G_c(N)$ is related analogously to the three principal values:

$$G_c(N) = \left[ \frac{N_1^2}{C_{c1}} + \frac{N_2^2}{C_{c2}} + \frac{N_3^2}{C_{c3}} \right]^{-1/2}. $$

This leads to an anisotropic cohesive law characterized by a direction dependent scaling along the traction axis and with constant characteristic opening displacement $D_c$. Fig. 6 illustrates the linearly decreasing cohesive law considered in the present application. An extension to more complex cohesive laws — where, e.g., the unloading branch is nonlinear or $D_c$ changes with the anisotropy direction — is straightforward.

The principal directions of anisotropy on the fracture plane are given by the axes of the ellipse resulting from the intersection of the resistance ellipsoid with the plane of normal $N$. In turn, the ellipse equation is the solution of the system

$$\frac{X_1^2}{T_{c1}^2} + \frac{X_2^2}{T_{c2}^2} + \frac{X_3^2}{T_{c3}^2} - 1 = 0, $$

$$N_1X_1 + N_2X_2 + N_3X_3 = 0. $$

The resulting equation can be expressed in a more compact form, by applying a rotation $R^N$ from the principal anisotropy system to the oriented surface and a in-plane rotation $R$ on the oriented surface to align with the principal ellipse axes. The decomposition of the rotation matrix is introduced here more for practical than for theoretical reasons, since rotations of the opening displacement components on the cohesive surface are requested during the calculations. Thus, the ellipse is expressed in the canonical form as:

$$\frac{U_1^2}{T_{cM1}^2} + \frac{U_2^2}{T_{cM2}^2} - 1 = 0, $$

where $U_1$, $U_2$ denote the intrinsic coordinates of the ellipse, i.e., the reference system in the center of the ellipse and with $U_i$ in the direction of $M_i$. The coefficients $T_{cM1}$ and $T_{cM2}$ in (8) define the maximum and minimum tractions reachable on the fracture plane. The orientations $M_1$ and $M_2$ of the anisotropy principal axes of resistance on the fracture surface in the reference system are recovered as

$$M_1 = R^N R^I_1, \quad M_2 = R^N R^I_2, $$

where $I_1 = \{1,0,0\}$ and $I_2 = \{0,1,0\}$ are the unit basis vectors in the reference of the local resistance ellipse on the cohesive surface. The maximum and the minimum cohesive strength are used to define the shear resistances along the orientations $M_1$ and $M_2$. For simplicity, we introduce a single parameter $\eta$, defined as the ratio between the maximum shear strength $\tau_{c\text{max}}$ and the maximum normal strength $T_{cM1}$ of the anisotropic material. The choice to use a unique parameter $\eta$ to define the shear strengths is dictated by the desire to reduce the number of input parameters. The assumption implies that the shear strengths on the cohesive plane scale according to an ellipse, proportionally to the normal strengths. Other choices, leading to more complicated resistance surfaces, can be made, but in general it is not easy to have information about all the strengths of an anisotropic material, therefore we comply with a simplified model. Thus, in our model the local shear strengths are derived as:

$$\tau_{c\text{max}} = \eta T_{cM1}, \quad \tau_{c\text{min}} = \eta T_{cM2}, $$

leading to the following definitions:

$$\beta = \frac{\tau_{c\text{max}}}{G_c(N)} = \eta \frac{T_{cM1}}{G_c(N)}, \quad \alpha = \frac{\tau_{c\text{min}}}{\tau_{c\text{max}}} = \frac{T_{cM2}}{T_{cM1}}. $$
The parameter $\beta$ in (9), measures the ratio between the maximum shear strength in the cohesive plane and the normal cohesive strength; it varies with the orientation of the cohesive surface. The parameter $0 \leq \alpha \leq 1$, in (9), also depends on the orientation and measures the ratio between the local minimum and maximum shear strengths on the cohesive surface. The introduction of the parameter $\alpha$ as the ratio between the in-plane shear resistances is done in order to recover easily the isotropic behavior of the cohesive surface described in the original formulation [24] by setting $\alpha = 1$. The definition (9) implies that the maximum and the minimum shear resistances on the cohesive plane scale with the tensile resistance. A more general model may adopt a different variation of the shear resistance with the orientation. In such a case, $\beta$ and $\alpha$ will additionally be functions of the direction on the cohesive surface.

Once the finite element discretization of the solid is performed, each inter-element surface is equipped with the three local cohesive parameters $T_c(N)$, $\beta$ and $\alpha$, and the two sliding directions $M_1$, $\delta_1$ and $M_2$, $\delta_2$. The local parameters derive from the three intrinsic anisotropic material strengths $T_{c1}$, $T_{c2}$, $T_{c3}$, and a single shear strength parameter $\tau_{cmax}$. As matter of fact, the normal strength $T_c(N)$ is computed through (6), which needs the three strengths $T_{c1}$, $T_{c2}$, $T_{c3}$. The two in-plane cohesive strengths $T_{cm1}$, $T_{cm2}$ are obtained through (7), or equivalently from (8), using the orientation of the orthotropy axis. Finally, (9) provides the value of the ratio $\eta$, used to compute the parameters $\alpha$ and $\beta$. In total, the cohesive model adopted here requires the assignment of four strength parameters (plus three orthotropy axes), and of the critical energy release rate $G_{c1}$.

4.2. Kinematics

The cohesive elements used here are isoparametric and with quadratic interpolation, therefore they may undergo a motion according to a two-curvature surface. Thus the kinematics has to be described through covariant and contravariant bases. This description is restricted to the cohesive surface, since the kinematics of the bulk is controlled by the logarithmic and exponential mappings.

Upon a motion defined by the mapping $\varphi(X)$, where $X$ are the material coordinates, the two originally coincident surfaces of a fracture may undergo different displacements. Let us denote with $\varphi^+$ the motion of the points of the two facing surfaces, respectively. The kinematics of the cohesive surface $S$ is defined by the separation, i.e., the displacement jump $\Delta$:

$$\Delta = \varphi^+ - \varphi^- = [\varphi]_S,$$

and by the motion of the mid-surface:

$$\varphi = \frac{\varphi^+ + \varphi^-}{2}.$$

The cohesive surface deformation gradient is defined as

$$\nabla \varphi_S = \frac{\partial \varphi}{\partial X}.$$

where $X$ are the material coordinates of the cohesive surface. Because we allow for arbitrary deformations and for general anisotropy of the cohesive surface it is mandatory to parametrize the cohesive surface and to define covariant and contravariant bases. Given a parametrization of $S$ by curvilinear coordinates $(s_1, s_2)$, the material basis vectors on the undeformed surface are given by:

$$A_1 = \frac{\partial X}{\partial s_1}, \quad A_2 = \frac{\partial X}{\partial s_2}, \quad A_3 = N = \frac{A_1 \times A_2}{|A_1 \times A_2|}.$$

Under the same parametrization, the current bases on the deformed $S$ is:

$$a_1 = \frac{\partial X}{\partial s_1}, \quad a_2 = \frac{\partial X}{\partial s_2}, \quad a_3 = n = \frac{a_1 \times a_2}{|a_1 \times a_2|}.$$

Both bases are written here in covariant form; their contravariant basis vectors are defined by duality, $A_i \cdot A^j = \delta_i^j$ and $a_i \cdot a^j = \delta_i^j$, respectively. Then, the cohesive surface deformation gradient follows directly from the definition of the derivative of a vector field in general coordinates [19]:

$$\nabla \varphi_S = a_2 \otimes A^2, \quad \alpha = 1, 2.$$

In the deformed configuration the anisotropic — in general non-orthogonal — material directions and the normal to the deformed surface are computed by

$$m_1 = \nabla \varphi_S \cdot M_1, \quad m_2 = \nabla \varphi_S \cdot M_2, \quad m_3 = n,$$

and the corresponding contravariant basis vectors are again defined by duality, $m_i \cdot m^j = \delta_i^j$. The displacement jump can now be described in either basis, using the contravariant or covariant components $\delta_i$ and $\delta_i$, respectively,

$$\Delta = \delta^1 m_1 + \delta^2 m_2 + \delta^3 n = \delta_1 m^1 + \delta_2 m^2 + \delta_3 n.$$
where
\[
\delta^i = \Lambda \cdot \bar{m}^i = A_i m_i^j, \quad \delta_j = \Lambda \cdot \bar{m}_j = A_j m_{ji}, \quad \text{and} \quad \delta^\alpha = \delta_{\alpha}.
\] (11)

In (11), \( A_i \) denote the Euclidian components of \( \Lambda \) (in the orthonormal reference basis \( E_i \)):
\[
\Lambda = A_1 E_1 + A_2 E_2 + A_3 E_3.
\]

### 4.3. Cohesive law and fracture criterion

In order to derive the cohesive law we adopt a thermodynamic point of view and define a free energy density per unit undeformed cohesive surface \( \Phi \), dependent on the mapping \( \varphi \) and on a set of internal variables \( \mathbf{q} \) attending irreversible processes:
\[
\Phi = \Phi(\varphi, \mathbf{q}).
\]

Assumptions of material frame indifference and independence on deformations (stretching and shearing) of the cohesive surface itself restrict the functional dependence of \( \Phi \) on the sole components of the displacement jump of the deformed system, cf. [24]. In our approach, we aim to derive a cohesive law expressed in the material framework, to comply with the choice of material stress and strain measures stated above. Given the relation (11) between material and spatial components of the displacement jump, we can write conveniently, with a slight abuse of notation:
\[
\Phi = \Phi(\delta^i(\Lambda), \delta_j(\Lambda), \delta^\alpha(\Lambda); \mathbf{q}) = \Phi(A_1, A_2, A_3; \mathbf{q}).
\]

The introduction of the two local cohesive parameters \( \beta \) and \( \alpha \), see (9), allows for the definition of an effective displacement jump \( \delta \) as:
\[
\delta = \sqrt{\beta^2(\delta^1)^2 + \alpha^2(\delta^2)^2} + (\delta^3)^2.
\] (12)

Note that \( \delta \) is a scalar, but its definition depends on the contravariant components of the displacement jump in the spatial configuration. It definition is not unique, since one can use the counterpart in covariant components. This second choice is an alternative, which would lead to a slightly different expression of the cohesive tractions. Let us now assume that the free energy density \( \Phi \) depends on the scalar displacement measure (12) only. Then the cohesive law provides an effective scalar traction in the spatial description by
\[
t = \frac{\partial \Phi(\delta, \mathbf{q})}{\partial \delta},
\]
while the effective cohesive stiffness in the spatial description follows by
\[
K = \frac{\partial^2 \Phi(\delta, \mathbf{q})}{\partial \delta^2}.
\]

The material cohesive tractions \( T_i \) and the material cohesive stiffness \( K^c_{ik} \) on the cohesive surface are computed through the chain rule (see Appendix A for the definition of the vector \( d_i \) and of the matrix \( D_{ij} \)) as:
\[
T_i = \frac{\partial \Phi}{\partial A_i} = \frac{t}{\delta} D_{ij} A_j, \quad K^c_{ik} = \frac{\partial^2 \Phi}{\partial A_i \partial A_k} = \left( K - \frac{t}{\delta} \right) d_i d_k + \frac{t}{\delta} D_{ik}.
\]

The operative form of the free energy density \( \Phi \) adopted in the present calculation agrees with the linearly decreasing law in Fig. 6 and reads:
\[
\Phi(\delta) = T_c \left( \delta - \frac{\delta^3}{2A_c} \right), \quad A_c = \frac{2G_c}{T_c}
\]
where \( T_c = T_c(\mathbf{N}) \).

In the framework of an adaptive finite element analysis, at the end of each loading step, once equilibrium has been reached, a failure test is carried out on every inter-elemental surface. To this end an effective traction \( t \), depending on the components of the traction vector acting on the cohesive surface, is computed and compared with the cohesive resistance associated to interface:
\[
t = \sqrt{(t^1)^2 + \beta^2[(t^2)^2 + \alpha^2(t^3)^2]} \leq T_c(\mathbf{N}),
\] (13)
where the contravariant spatial components of the tractions on the cohesive surface are computed from the material traction vector \( T \) as:
\[
t^i = T \cdot m^i = T_i m_i^j.
\]
If the criterion (13) is violated, the topology of the mesh is updated with the insertion of a new surface according to the algorithm described in [26]. Note that for general mixed mode analyses it is incumbent according to the condition (13) to account for both normal and shear components of tractions.

In a finite element implementation, the cohesive energy depends on the nodal displacements not only through the opening displacement, but also through the orientation of the principal orientations \( m_1, m_2 \) and \( n \). This dependence appears explicitly in the computation of the tangent stiffness, which accounts for the current geometry of the cohesive surface. The derivatives of \( \delta \) with respect to the basis vectors can be found in Appendix A. The full expressions of the nodal forces and of the consistent tangent stiffness are reported in Appendix B. The versatility of the general anisotropic cohesive approach is illustrated in the following section by means of numerical examples of failure in silicon dies.

5. Fragmentation of silicon dies

In order to get some deeper insight in the failure modes of the silicon dies, we performed several finite element analyses of the BoE experiments described in Section 2. The reduction of the average strength and the increase of the strength dispersion seems to be associated to the presence of localized damage on the zones where the maximum stress is achieved during the BoE test, i.e., on the edges and at the surface around the loading sphere. Note that we do not aim here to perform a systematic study of the failure mechanisms of the silicon plates, but to achieve an understanding of the possible causes of mechanical failure of the plates. In particular, we want to identify the reasons of a reduced global resistance of the material.

Unfortunately, we do not have any information about the actual material properties of the tested silicon die batch. The elastic properties of the bulk material used in the numerical calculations are given in Section 3. The material parameters for the fracture simulations are listed in Table 1; such values have been recovered from the literature [13,20,22,29,32]. It is important to observe that the choice of the material parameters justifies the mismatch between the failure loads measured in the experiments and in the subsequent numerical calculations.

The only parameters not recoverable from the literature were the three anisotropic critical energy release rates \( G_{c_i} \). A unique value was tuned by preliminary numerical experiments, that allowed us to determine the order of magnitude of the maximum \( G_{c_3} \). The other critical energy release rates were obtained by scaling, making them proportional to the cohesive strengths, according to the simplified model described in Fig. 6.

The silicon die is meshed with 10-node tetrahedral elements. We need to emphasize that a numerical simulation of brittle fracture and fragmentation in a quasistatic setting requires the computation of a sequence of non-equilibrium states. Such finite element analyses, which we performed here by recourse to a dynamic relaxation technique [34,23] in combination with the adaptive fragmentation algorithm, lead to rather expensive computations. For this reason in the fragmentation analyses the meshes of the plates are relatively coarse; they have about 15,000 nodes and an average mesh size \( h = 0.075 \) mm. Much finer meshes would be required to completely resolve the cohesive zone size, which, for the current material properties is approximately:

\[
L \approx \frac{E}{1 - \nu^2} \frac{G_c}{T_c} = 0.0015 \text{ mm.}
\]

Fracture analyses with such a fine discretization were impractical for our study, they would call for a parallelized version of finite element code. Analyses with coarser meshes, on the other hand, clearly go on cost of the accuracy of the computation and on its reliability from the quantitative standpoint.

Also for reason of efficiency, we choose not to model the full contact problems of the bearing and loading spheres, but employ instead a displacement controlled loading in predefined, limited zones. The setup has been checked thoroughly by means of purely elastic – both isotropic and anisotropic – analyses of the whole BoE geometry. Fig. 7 shows the load-deflection curves computed in two elastic, anisotropic BoE analyses with different loading conditions in order to validate the simplified loading and boundary conditions employed in the subsequent fracture analyses. We observe that the simplification on the boundary conditions affects the plate behavior which shows a stiffer behavior, but not the location of the maximum stress. The highest tensile stresses localize at the posterior side of the limited loaded zones, and cracks develop from those location. In a fracture analysis, the change of the boundary condition will affect in general the failure load, but not the location of the fracture nucleation and the subsequent evolution of the crack.

For the failure analysis, here we present the results obtained with two different meshes, one with a uniform mesh size and the second one with a refinement of the elements in proximity of the loaded edge in order to better capture edge effects, Fig. 8. The meshes are unsymmetric because they have been generated in a random way. In both meshes, a straight middle line is included to enforce symmetry in the geometry of the loading. The first mesh shows a certain degree of symmetry.

Table 1

<table>
<thead>
<tr>
<th>( T_{c_1} ) (MPa)</th>
<th>( T_{c_2} ) (MPa)</th>
<th>( T_{c_3} ) (MPa)</th>
<th>( \eta ) ((^{-}))</th>
<th>( G_{c_1} ) (N/mm)</th>
<th>( G_{c_2} ) (N/mm)</th>
<th>( G_{c_3} ) (N/mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>1000</td>
<td>1500</td>
<td>1</td>
<td>0.007</td>
<td>0.007</td>
<td>0.0105</td>
</tr>
</tbody>
</table>
because of the equi-distance of the nodal points, while the second one possesses a higher degree of randomness. The second mesh is refined in order to allow for the introduction of small local defects.

5.1. The flawless silicon die

In a first analysis we assume the material to be flawless, characterized by the ideal elastic properties of Section 3, and by a uniform isotropic in-plane strength of 1000 MPa.

In order to allow for arbitrary crack patterns we meshed the die uniformly with a mesh size, as already mentioned, of $h = 0.075$ mm. Although a few microcracks develop at the loading point since the beginning of the analysis, they grow very slowly so that they do not reduce sensibly the global stiffness of the die. The die bends up to a maximum displacement of 0.2 mm which corresponds to a loading of about 45 N. This is clearly higher than the failure load measured in the experiments. Subsequently the microcracks starts to coalesce and to propagate toward the edge and the stiffness drops. Thus the crack propagates in the opposite direction along a quite straight path; the final configuration is visualized in Fig. 9. The analysis shows that it is correct to account for the full non-linearity of the problem: before cracking the silicon die undergoes a deflection larger than its thickness.

In commenting the fracture analysis of the flawless case, we would like to mention that in preliminary analyses we have used two other meshes, besides the one presented here, with a different degree of refinement: a coarser mesh and a finer mesh. The resulting crack patterns were similar, but differences were observed in terms of global resistance, higher for the coarser mesh, smaller for the finer mesh. Unfortunately, the finer mesh did not go completely through, because of endless computation times, and we got only a small portion of the crack. Therefore an estimate of the final crack pattern was not achieved. The partial results confirmed the observations of our previous work [12] and are in keeping with the general results concerning mesh dependency in isotropic materials.
5.2. Weakened surface of the die

The failure fractures observed in the experiments are characterized by more complex patterns than the ones provided by the numerical simulation of the flawless die and, moreover, the chip fails at lower load. One reason for that are flaws and scratches at the surface induced during the processing phase. The effect of machining suggests a general uniform damaging of the surface of the dies, and the simplest way to account for this damage in elastic-brittle materials is to assume a reduction on the elastic stiffness. This assumption is inherited from classical damage mechanics. It is likely that the maximum damage due of machining will be observed across the thickness and therefore we decide to reduce the out-of-plane elastic modulus. Regrettably this assumption has been confirmed only by the numerical results, and it cannot be supported directly by the experimental data. In fact, the experimentalists did not provide information about the dependence of the stiffness of the materials on the machining, neither load-displacement curves that we can use for a direct evaluation of the stiffness reduction, since the experiments were performed in order to derive a statistical correlation between damage induced by the machining of the die batch and the observed failure mechanism.

The reduction of 15% the out-of-plane elastic modulus has been chosen through the execution of a couple of preliminary analyses. Smaller reductions, less than 10%, do not have sensible effects, while bigger reductions, greater than 20%, lead to unrealistic material properties for the considered silicon. The anisotropic fracture properties are listed in Table 1.

Let us remark that a reduction of the cohesive properties alone, tried in our numerical experiments up to 30%, does not reproduce realistic results. In fact, initially we tried to simulate the edge flaw by reducing the cohesive strength in proximity of the loading area, but this produced unrealistic fracture patterns. For a small strength reduction, the fragmentation patterns are straight cracks, as in Fig. 9. For a 30% or larger strength reduction, the failure is characterized instead by hole-like fragments but no propagating cracks are observed. Note that this behavior manifests also if isotropic cohesive properties are adopted. Obviously the etching of the chip on top of the die is a process which, effectively, weakens the whole structure, and a reduction of the stiffness seems to be more appropriate to reproduce this kind of damage.

5.3. Weakened edge of the die by defects

Although closer to the experiments, the numerical crack patterns obtained with a reduced stiffness of the material were not able to describe the formation of large fragments. The fact that cracks deviate from their initial direction and link to produce fragments may be related to the anisotropy of the material as well as to the presence of local defects due to the cutting along the edges. Local edge imperfections in silicon die can be observed easily with a microscopy. These defects define the onset of failure and suggest preferential paths for cracks. Thus, we performed another analysis with a mesh refined in proximity of the support points, see Fig. 8b. The mesh had to be refined in order to introduce small local defects. In order to model small edge defects, we induce a notch by simply disconnecting two finite elements at the front edge.

Now the die starts to crack earlier, i.e., at an applied displacement which corresponds to a load of about 10 N. Cracks develop from the bearing points and link forming large size fragments. Clearly, the presence of several elements across the thickness and the anisotropy in strength allows here for the formation of quite different cracks patterns, see Fig. 11. Note that the pattern in Fig. 11 is unsymmetric. In fact, the right side splits into a big fragment, while the left side is still connected to the remaining part of the plate and shows a quite strong bending. We observe that this case is characterized by a local

---

Fig. 9. Fracture pattern evolution as obtained in a fracture finite element simulation of the BoE test, assuming high stiffness and the nominal strength for the material (flawless material).
damage on the edges – which activates three cracks instead of a single one – but the stiffness of the material is everywhere high.

5.4. Comparison

The comparison between the responses of the three models involve on a side the crack patterns, and on the other side the global behavior in terms of load-displacement curves.

We start by observing that the same mesh has been used for the flawless and for the weakened surface silicon dies. The sole difference in the two analyses is the out-of-plane stiffness. Clearly, the moderate unsymmetry of the mesh affects the crack path in both the analyses, and this point would be worth to be investigated in a deeper way. Anyhow, here we achieved an important result that we aimed to obtain, i.e., when there is a general weakening of the stiffness due to the machining, the die breaks with a different mechanism. The explanation is that in a more compliant anisotropic material the elastic response globally changes, inducing a different stress distribution. In the particular case here examined, the stress change leads to the evolution of two crack branches, instead of the formation of a unique, almost straight crack. Later on, one of the cracks can arrest – see the right side – or continue propagating – see the left side -. After branching, the mesh will play a fundamental role to define the correct path of the cracks, but the branching seems to be dictated by the initial elastic stress state. Such double behavior, flawless and uniformly flawed, can only be captured by an anisotropic model, where only one of the three elastic moduli can be manipulated. In an isotropic model, instead, the reduction of the unique elastic modulus will affect all the stress components proportionally.

The different patterns correspond to different global resistances of the plates. For the three cases of Figs. 9–12 shows the plots of the reaction force to the pushing ball versus the vertical displacement of the loading point.

We remark that all the analyses are characterized by the onset of cracks under the pushing ball at the first loading steps and, therefore, the initial part of all the load-displacement curves is not a straight line. The development of the initial pattern of cracks, however, is different in all three cases and so is the global response. As expected, it is observed that in the
uniformly flawed case the average failure load is below the value provided by a flawless material. The initial response is also more compliant, i.e., a reduction of about 11% of the apparent stiffness between the flawless and the uniformly flawed model can be noted. Moreover, it appears clearly that in the edge flaw case the initial crack induces less local damage than in the homogeneous cases, revealing a bigger stiffness in the global response. While for the flawless and uniformly flawed plates cracks advance continuously, in the other case the edge flaw causes the formation of two additional cracks starting, shortly later on, from the edge. Although in the edge flaw case three cracks are present, they propagate slower than in the other cases. Our explanation is that the three cracks somehow compete modifying the stress field, rendering it more homogeneous and reducing the amount of local damage. The reduction of the global stiffness manifests only when the central crack reaches the edge and the resistance of the plate drops. Some additional difference in the initial stiffness may be also introduced by the two distinct meshes.

The edge flaw curve does not show any dominant peak in the initial part. This seems to suggest that the localization of damage allows the propagation of cracks that dissipate a good part of the loading work, leaving less energy available to deform the plate elastically; thus the reaction is lower. Later, the reaction for the edge flaw case remains constant, indicating a uniform and stable propagation albeit not along a straight path. Finally, large fragments form and lead to the steep and quick reduction of the global reaction.

We conclude this section with three final comments. The fundamental reason for the adoption of an anisotropic cohesive model is that the actual material is anisotropic, but it could be interesting to see how closely an isotropic model can reproduce the behavior of the silicon under BoE tests. Indeed, in the phase of setting the uniform mesh model, we performed preliminary analyses considering an isotropic material to model both elastic and brittle behaviors of silicon. While the difference in terms of elastic response was modest, the difference in the fracture response was instead remarkable. In particular, if the cohesive strength \( T_{c3} \) was reduced, or set equal to the other two normal strengths, unrealistic fracture patterns formed, characterized by hole-like fragments in proximity of the loaded area, and no propagating cracks were observed.

Mesh dependency is expected in terms of quantitative results, but we decided not to address this point within the present research, for two main reasons. First, the simulations take a lot of time and the gain of information will not pay for the improvement of the results, given the quite large uncertainty of the input data. Second, the more the mesh is refined, the more precisely the load boundary conditions will need to be enforced, making the use of contact algorithms mandatory. In fact, with a very fine mesh the loading sphere will produce plenty of tiny fragments that need to be controlled against interpenetration. This makes the analyses prohibitive for the current sequential version of the algorithm.

It is important to observe that the strength values used in the calculation, and retrieved from the literature, are characterized by a large scatter, even as high as 70% of the average value. The variability of the resistance surely affects the propagation of cracks, since it will enhance local anisotropy and inhomogeneity. The influence of the strength scatter on the overall behavior of silicon dies is a difficult task to be investigated. To account for variability of the strength, we should abandon the deterministic approach used here, and switch to a probabilistic approach, setting up a wide program of calculations by using, for example, the Montecarlo method. In a statistic approach, the scatter of the strength may be considered as one of parameters governing the crack pattern and the global resistance of the silicon dies, and it might help in justifying the different failure modes observed in the experiments. This is in our plans for the future, but this can be only done when a concurrent version of the code will be available, since the anisotropic calculations combined with fracture propagation are very time consuming.

![Fig. 12. Vertical reaction versus vertical displacement for the three analyses of Section 5.](image-url)
6. Conclusions

In order to get a deeper insight into the failure mechanisms of silicon dies, we developed a general technique for anisotropic fracture analysis by finite elements. The discretized plates undergoing a fracture process are studied by means of cohesive theories. The discretized models are originally fully coherent and cohesive elements are introduced only when the fracture criterion (13) is fulfilled. Experiments showed that only a few dies in a specimen batch fail with a single straight crack traversing the plate, to which corresponds a high failure load denoting a high quality material. Reasons for different behaviors, showing meandering paths and fragment formation, may be due to the presence of distributed microcracks on the die’s surface or notchings effects of scratches along the edges.

Our numerical simulations are able to capture qualitatively such effects and allow for a comparison of the different mechanisms of failure for silicon dies. We can state that failure patterns characterized by cracks crossing the whole specimen, eventually characterized by several branches, are typical of a diffused damage that can be represented by a reduced out-of-plane stiffness of the die. On the other hand, the presence of local edge defects induces multiple cracks, more likely to link and to lead to the formation of fragments below the loaded zone, which reduces significantly the failure load, as observed experimentally.

In conclusion, with the technique introduced here, the qualitative macroscopic effects of anisotropy on the propagation of fracture can be captured. However, in order to perform systematical studies of fragmentation, to quantify their correlation to the failure strength, and to rule out any mesh dependency effects, we need a strong improvement of the numerical calculation, to be realized, e.g., by a parallelization of the code.

Acknowledgements

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Appendix A

The derivatives of the effective opening displacement (12) with respect to the components \( A_i \) are:

\[
\frac{\partial \delta}{\partial A_i} = \frac{1}{\sigma} \left[ \beta^2 (m_i^1 m_i^1 + \sigma^2 m_i^2 m_i^2) + n_i n_k \right] A_k = \frac{1}{\sigma} D_{ik} A_k = d_i.
\]

The second derivatives are:

\[
\frac{\partial^2 \delta}{\partial A_i \partial A_j} = \frac{1}{\sigma} (D_{ij} - d_i d_j).
\]

The derivatives of the effective opening displacement (12) with respect to the basis vector components are:

\[
\frac{\partial \delta}{\partial m_i} = \frac{1}{\sigma} A_i \delta^i, \quad \frac{\partial \delta}{\partial m_i^1} = \frac{1}{\sigma} \beta^2 A_i \delta^1, \quad \frac{\partial \delta}{\partial m_i^2} = \frac{1}{\sigma} \beta^2 A_i \delta^2,
\]

Therefore, the derivatives of the cohesive tractions (13) with respect to the deformed basis vectors are expressed as:

\[
\frac{\partial T_i}{\partial m_i^1} = \beta \left[ \left( K - \frac{t}{\delta} \right) \frac{\delta^1}{\sigma} d_i \otimes A_j + \frac{t}{\delta} (m_i^1 A_j + \delta^1 \delta_{ij}) \right],
\]

\[
\frac{\partial T_i}{\partial m_i^2} = \beta^2 \left[ \left( K - \frac{t}{\delta} \right) \frac{\delta^2}{\sigma} d_i \otimes A_j + \frac{t}{\delta} (m_i^2 A_j + \delta^2 \delta_{ij}) \right],
\]

\[
\frac{\partial T_i}{\partial m_i^3} = \left( K - \frac{t}{\delta} \right) \frac{\delta^3}{\sigma} d_i \otimes A_j + \frac{t}{\delta} (n_i A_j + \delta^3 \delta_{ij}).
\]

Appendix B

Assume the nodal displacements \( U_{ai} \) as variables of the finite element approximation. The displacement field in Euclidian components is described as:

\[
u_i = \sum_a N_a U_{ai},
\]

where \( N_a \) is the shape function for the node \( a \). The displacement jump and its derivatives with respect to the nodal displacements are expressed as:

\[
\text{Appendix A}
\]

\[
\text{Appendix B}
\]
The consistent tangent stiffness for the nodes $A_i = \sum_n N_n (U_{ij}^* - U_{ij}), \quad \frac{\partial A_i}{\partial U_{ij}} = \pm N_b \delta_{ij}.$

The cohesive surface coordinates and derivatives become:
\[ \hat{x}_i = \sum_n N_n x_{i\alpha} + \frac{1}{2} N_n (U_{ij}^* + U_{ij}), \quad \frac{\partial \hat{x}_i}{\partial U_{ij}} = \pm \frac{1}{2} N_n \delta_{ij}. \]

The undeformed and deformed surface basis vectors are computed as:
\[ A_{ij} = \frac{\partial \hat{x}_i}{\partial x_j} = \sum_n \frac{1}{2} N_n (x_{i\alpha} + x_{i\alpha}^*), \quad a_{ij} = \frac{\partial x_i}{\partial x_j} = \sum_n \frac{1}{2} N_n x_{i\alpha}^*. \]

and their derivatives with respect to the nodal displacements are:
\[ \frac{\partial A_{ij}}{\partial U_{ij}} = 0, \quad \frac{\partial a_{ij}}{\partial U_{ij}} = \frac{1}{2} N_b \delta_{ij}. \]

The dual basis vector components $A^\beta_i$ in the reference configuration are obtained from (15), using the following relationships:
\[ A^1 = \frac{A_2 \times N}{A_1 \cdot (A_2 \times N)}, \quad A^2 = \frac{N \times A_1}{A_2 \cdot (N \times A_1)}, \quad A^3 = \frac{A_1 \times A_2}{N \cdot (A_1 \times A_2)}. \]

The deformed basis vectors $(n, m^\beta, \beta = 1, 2, \text{sum over } \alpha)$ and their derivatives are:
\[ n_i = \frac{\epsilon_{\alpha \beta \gamma} n_{(i)\beta}}{\alpha_1 \times a_2}, \quad \frac{\partial n_i}{\partial U_{ij}} = \frac{\epsilon_{\alpha \beta \gamma}}{2(a_1 \times a_2)} (n_{\alpha 1} N_{\alpha 2} - a_{28} N_{a 1}) (\delta_{ij} - n_{i} n_{j}) = R_{i\beta}, \]
\[ m_i^\beta = a_{\alpha 1} A_{\alpha 1}^\beta M^\beta_1, \quad \frac{\partial m_i^\beta}{\partial U_{ij}} = \delta_{ij} \frac{1}{2} N_{\alpha 3} A_{\alpha 1}^\beta M^\beta_1 = \delta_{ij} R_{i\beta}^\gamma. \]

The total free energy density over a cohesive element of surface $\Omega_b$ is given by
\[ \phi^\sigma = \int_{\Omega} \phi(\delta) d\Omega. \]

The components $I$ of the nodal forces at the node $a$ are computed as:
\[ F_{ai}^\sigma = \frac{\partial \phi^\sigma}{\partial U_{ai}} = \int_{\Omega} \frac{\partial \phi}{\partial U_{ai}} \frac{\partial A_i}{\partial U_{ai}} d\Omega = \int_{\Omega} T_i N_a d\Omega. \]

The consistent tangent stiffness for the nodes $a$ and $b$, components $I, J$ derives as:
\[ K^\sigma_{aij} = \frac{\partial F_{ai}^\sigma}{\partial U_{aj}} = \int_{\Omega} \left[ \frac{\partial^2 \phi}{\partial U_{ai} \partial U_{aj}} \frac{\partial A_i}{\partial U_{ai}} + \frac{\partial T_i}{\partial U_{ai}} \frac{\partial m_{\beta}^\beta}{\partial U_{aj}} + \frac{\partial T_i}{\partial m_{\beta}^\beta} \frac{\partial A_i}{\partial U_{aj}} + \frac{\partial T_i}{\partial m_{\beta}^\beta} \frac{\partial A_i}{\partial U_{ai}} \right] d\Omega \]
\[ = \int_{\Omega} \left[ K^\gamma_{bj} N_b N_a d\Omega + \int_{\Omega} \left[ \frac{\partial T_i}{\partial m_{\beta}^\beta} R_{bj} \frac{\partial A_i}{\partial U_{ai}} + \frac{\partial T_i}{\partial m_{\beta}^\beta} R_{bi} \frac{\partial A_i}{\partial U_{ai}} + \frac{\partial T_i}{\partial m_{\beta}^\beta} R_{bj} \frac{\partial A_i}{\partial U_{ai}} \right] d\Omega \right] N_a d\Omega. \]

In the case of isotropic behavior, the expressions reported in [24] are recovered.

References


