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A novel monolithic approach for modelling crack propagation

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Résumé — A new finite element method is explored to model crack propagation in a silicon substrate bonded with a stress-inducing layer. This approach is based on the level-set method coupled with anisotropic remeshing to define the crack faces and tip. Furthermore, the $G\theta$ method is used for computing the strain energy release rate and the propagation direction. Simulations are performed in a monolithic Lagrangian framework.

Mots clés — crack propagation, mesh adaptation, $G\theta$ method, monolithic approach

1 Introduction

Solar energy is considered as one of the most interesting sustainable form of energy. It is however still insufficiently used due to the high price of solar panels. A significant part of the cost depends on the thickness of the silicon wafer integrated to the solar panel [1]. Using a thin silicon layer, the solar panel becomes more efficient with a maximal efficiency limit reached for a silicon thickness ranging between 40 and 60 μm [2].

During the last decade, many studies concentrated on the development of a process for manufacturing very thin silicon wafers while reducing material loss. One of the most interesting ways to produce such wafers is based on the fracture mechanism of silicon. The basic idea behind this new concept is to induce a controlled failure of silicon by a tensile stress field produced by another layer called "stress-inducing layer" bonded with the silicon substrate. The lift-off differs from one process to another by the nature of the stress-inducing layer and the manner to introduce the stress field. For example, the glue cleave method [3] proposes using a metallic stress-inducing layer glued under a pre-cracked silicon one and allows getting a 180 μm -thick layer of silicon. In this process, the matter is pulled down by a force during the cooling stage while the silicon layer is held fixed firmly. This method gives good results. However, thinner layers are required to reach the maximal efficiency of solar panels. Another recent process introduced by Bedell *et al.* [4] and simulated by Bouchard *et al.* [5] is dedicated to this objective. In their method the stress-inducing layer, made of Nickel, is deposited using electroplating or electro-less plating techniques and an additional flexible adhesion layer is applied to the top of the metal layer. By pulling on this adhesive layer, the crack propagates in a controllable manner, parallel to the interface.

Another very promising approach called the 'SLiM-Cut' process takes advantage of the difference in the thermal expansion coefficient between an epoxy stress-inducing layer and the silicon substrate during cooling [2]. The propagation occurs by the fact that the stress-inducing layer, having a higher thermal expansion coefficient than the silicon's, is deposited and bonded on the silicon substrate. A static sensitivity analysis of the geometrical and mechanical characteristics of the stress-inducing layer and the silicon substrate on the stress intensity factors (SIF) and the crack's propagation direction was performed in the works of Toufayli *et al.* [7].

In this paper, a dynamic crack propagation modelling for the SLiM-Cut process is performed. This crack propagation phenomenon is based on the level-set method, anisotropic remeshing and on a novel method for choosing the Lagrangian convection velocity. In the second section, the SLiM-Cut process is described along with a review of Toufayli *et al.*'s [7] important results. The third section is dedicated to the numerical modelling of the process where the basics of the crack propagation technique are detailed.

And the fourth section is the conclusion of this paper.

All numerical calculations mentioned in this paper were performed with the CimLib finite element C++ library [8].

2 The SLiM-Cut process

The SLiM-Cut process, invented by IMEC [1], is a process based on fracture mechanics concept to produce a thin silicon wafer by slicing a parent substrate of mono-silicon under thermal cooling. The development of this process aims at reducing material loss that results from using conventional wire sawing processes together with a reduction of the silicon wafer's thickness. This method is based on thermo-mechanical treatments : a high stress field is induced in a silicon substrate ; a crack propagates along the silicon substrate parallel to the interface with the stress-inducing layer. The top silicon layer is separated from the parent substrate and processed into a solar cell after a cleaning stage. The silicon substrate can be re-used for a new SLiM-Cut process. This method consists of the following steps :

- A stress-inducing layer, having a stronger interface during the warm up phase and a higher thermal expansion coefficient than the silicon's, is deposited and bonded at high temperature on a silicon substrate.
- During the cooling phase, the silicon layer experiences high stress levels due to the difference in thermal expansion coefficients. When this stress exceeds the fracture toughness of silicon, a crack initiates and propagates in a direction parallel to the surface of the substrate.
- A cleaning step dissolves most of the stress-inducing layer.
- Finally, the parent wafer is conditioned to be re-used in the first step.

Figure 1 illustrates the 2D geometry of the SLiM-Cut model where a rectangular shape silicon substrate is covered with a stress-inducing layer. In this figure, h_{Si} , l_{Si} are the thickness and the length of the silicon substrate respectively and h_l is the thickness of the stress-inducing layer. Also, a and d correspond, respectively, to the crack length and depth beneath the interface.

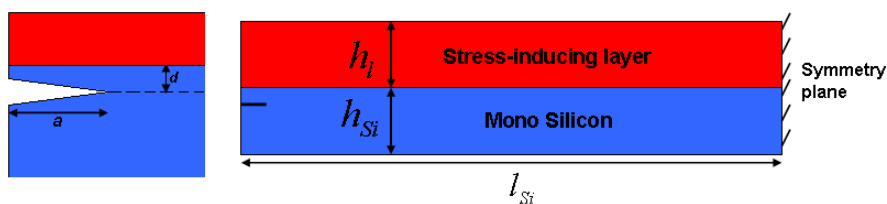


Fig. 1 – 2D Geometry of the SLiM-Cut model

Tables 1 and 2 sum-up the thermo-mechanical properties of the epoxy and the silicon respectively [6].

Property	Unit	Value
Young modulus (E)	MPa	19000
Poisson ratio (μ)		0.18
Density (ρ)	$Kg.m^{-3}$	1750
Thermal conductivity (K)	$W/(m.K)$	0.6
Thermal expansion coefficient (α)	$10^{-6}K^{-1}$	20
Heat capacity (C_p)	$J/(K.Kg)$	900

Tableau 1 – Thermo-mechanical properties of the epoxy

As mentioned in the introduction, a parametric study of the SLiM-Cut process was performed in [7]. In this study the initial temperature was fixed to 413K, the final cooling temperature to 100K with a heat transfer coefficient of $193W/(m^2.K)$. After studying the influences of the pre-crack length, the epoxy and the silicon thicknesses on the SIF and the propagation direction, it was concluded that for an initial crack length $a = 1.5mm$ at a depth $d = 50\mu m$, a silicon thickness equal to $h_s = 0.6mm$ and an epoxy

Property	Unit	Value
Young modulus (E)	MPa	130000
Poisson ratio (μ)		0.278
Density (ρ)	$Kg.m^{-3}$	2329
Thermal conductivity (K)	$W/(m.K)$	156
Thermal expansion coefficient (α)	$10^{-6}K^{-1}$	2.616
Heat capacity (C_p)	$J/(K.Kg)$	713
Fracture toughness (K_{Ic})	$MPa.\sqrt{mm}$	31.6

Tableau 2 – Thermo-mechanical properties of the silicon

thickness of $h_l = 0.3mm$, the crack will begin propagating horizontally after 2.3 seconds of cooling. These pre-mentioned parameters are used in the remainder of this paper.

3 Numerical modelling of the SLiM-Cut process

3.1 Level-set and mesh adaptation

In the perspective of modelling crack propagation in the silicon during the SLiM-Cut process, a monolithic approach with a Lagrangian framework is used. The monolithic method consists in using a unique mesh in which the different domains (i.e. silicon and epoxy) are considered using a level-set function. Consequently, different structures are immersed in a larger domain of different material properties so that boundary conditions at the interface can be replaced naturally. Furthermore, the level-set function, defining the silicon/epoxy interface, is used to mix the different thermo-mechanical properties of the silicon and the epoxy using appropriate mixing laws [9, 10]. Moreover, this function is used for meshing and remeshing operations in order to describe properly the considered interface and also to take into account the discontinuities of the physical properties. Mesh adaptation is also needed at the crack tip to insure the computational accuracy of the singular fields. It has to be noted that, contrary to XFEM, these singular fields are not imposed in the shape functions of the elements containing the crack tip.

To this end, it is crucial to pre-adapt anisotropically the mesh at the silicon/epoxy interface, the crack faces and tip. By doing so, the mesh becomes locally refined, elements are stretched, which enables to sharply define the interface and to save a great number of elements compared to classical local isotropic refinement. This anisotropic adaptation is performed by constructing a metric map controlled by a directional error estimator based on local interpolation error of the wanted fields which are in this case the level-set functions defining the silicon/epoxy interface and the crack faces and the pressure field. Furthermore, in our case, three different metrics are obtained, one for each field. The intersection of these metrics [11] leads to the one used for mesh adaptation.

In the goal of constructing these metrics, an *a posteriori* error estimator [12] is used. This error estimator uses the eigenvalues and eigenvectors of the recovered Hessian matrix of a given function and a wanted number of elements to construct the metric field. In practice, the mesh is generated in several steps using the MTC mesher and remesher developed in [13]. The proposed mesh generation algorithm works well for 2D or 3D complex shapes. It allows the creation of meshes with extremely anisotropic elements stretched along the interfaces. The mesh size is then only refined in the direction of the high physical and mechanical properties gradients. This allows both conserving a high precision in the computations and in the geometry description. During propagation, the mesh is only modified in the vicinity of the interface and near the crack tip which keeps the computational work devoted to the mesh generation low.

Figure 2 shows the result of this technique on the construction of the initial mesh and its effect on the computation of the normal stress at the crack tip.

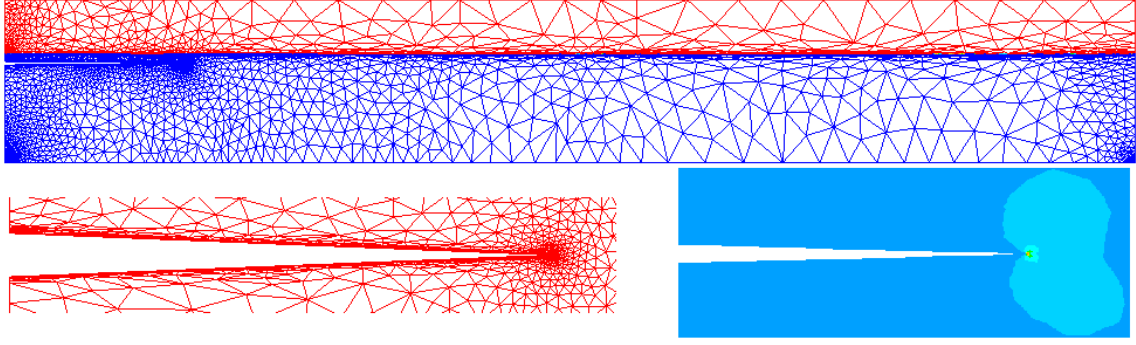


Fig. 2 – (a) Initial state of the SLiM-Cut process, (b) anisotropic meshing adaptation based on an *a posteriori* error estimation and (c) σ_{yy} at the crack tip

3.2 Governing equations

After mixing the different thermo-mechanical properties, thermal resolution is firstly performed using a stabilized convection diffusion solver. The thermal problem is written :

$$\begin{cases} \rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{v} \nabla T \right) - K \Delta T = 0 & \text{on } \Omega \\ -K \nabla T \cdot \mathbf{n} = h(T - T_{end}) & \text{on } \Gamma \setminus \Gamma_r \\ -K \nabla T \cdot \mathbf{n} = 0 & \text{on } \Gamma_r \end{cases} \quad (1)$$

where T is the temperature, T_{end} is the final cooling temperature, \mathbf{v} is the velocity, \mathbf{n} is the outward normal vector, Ω is the computational domain, Γ is the whole domain's boundary and Γ_r is the right boundary of the domain.

Afterwards, the thermo-mechanical problem is written using the Boussinesq approximation. The resolution of this problem is realized thanks to a stabilized mechanical multi-fluid solver, able to handle high thermophysical property discontinuities. A compressible linear isotropic elastic formulation is used. Finally, the subsequent system is solved :

$$\begin{cases} \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \nabla \mathbf{u} \right) - \nabla \cdot (2\mu \Delta \boldsymbol{\varepsilon}(\mathbf{u}) - p\mathbf{I}) = \rho(1 - \alpha(T - T_{end})) \mathbf{g} & \text{on } \Omega \\ \nabla \cdot \mathbf{u} + \frac{1}{\chi} \frac{dp}{dt} = 0 & \text{on } \Omega \\ \mathbf{u} = 0 & \text{on } \Gamma_b \\ \mathbf{u} \cdot \mathbf{n} = 0 & \text{on } \Gamma_r \end{cases} \quad (2)$$

where \mathbf{u} is the displacement, $\mu = \frac{E}{1+\nu}$ is the first Lamé coefficient, χ is the compressibility coefficient, \mathbf{g} the acceleration due to gravity, p is the pressure, $\boldsymbol{\varepsilon}(\mathbf{u})$ is the strain tensor and Γ_b is the lower boundary of the domain.

3.3 Crack propagation

3.3.1 Computing the strain energy release rate

The strain energy release rate G represents the energy required for a unitary crack increase. The criterion states that among all virtual and kinematically admissible crack propagation directions, the real increase is the one which maximizes the strain energy release rate. The kinking angle, θ_0 , is then determined by :

$$\begin{cases} \left(\frac{dG}{d\theta} \right)_{\theta=\theta_0} = 0 \\ \left(\frac{d^2G}{d\theta^2} \right)_{\theta=\theta_0} \leq 0 \end{cases} \quad (3)$$

Numerous numerical techniques can be used to compute G [14]. In this study, the $G\theta$ method [15] is used. It consists in defining two paths C_1 and C_2 around the crack tip. These paths divide the domain near the crack tip into three sub-domains (see figure 3).

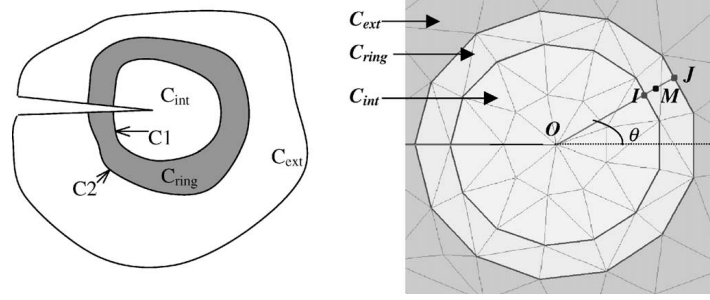


Fig. 3 – Contours and domains used to compute G with the $G\theta$ method [14]

Afterwards, the strain energy release rate computation is performed by solving :

$$G = \int_{C_{ring}} \left[Tr(\sigma \nabla \mathbf{u} \nabla \Theta) - \frac{1}{2} Tr(\sigma \nabla \mathbf{u}) \nabla \cdot \Theta \right] dC_{ring}. \quad (4)$$

where $Tr(\cdot)$ is the trace operator, σ is the stress tensor and Θ (vector) is a virtual unit displacement field in the θ (angle) direction.

3.3.2 Convection velocity and results

The computation of G infers the calculations of the propagation direction, θ_0 and the speed at the crack tip, \dot{a} . This speed is bigger than zero only if $G \geq G_c$ where G_c is the fracture energy in function of K_{Ic} . Hence, a velocity at the crack tip, \mathbf{v}_{ct} , can be given by :

$$\mathbf{v}_{ct} = \dot{a}(\cos\theta_0, \sin\theta_0). \quad (5)$$

This velocity insures the proper propagation of the crack but not the crack opening. The latter can be insured by the mechanical velocity, \mathbf{v} . These facts lead us to use a Lagrangian convection velocity which is the combination of \mathbf{v}_{ct} and \mathbf{v} . This convection velocity, called \mathbf{v}_{convec} , is given by :

$$\mathbf{v}_{convec} = \begin{cases} \mathbf{v} & \text{if } \dot{a} = 0 \iff G < G_c \\ \mathbf{v}_{ct}(H(\beta)) + \mathbf{v}(1 - H(\beta)) & \text{if } \dot{a} \neq 0 \iff G \geq G_c \end{cases} \quad (6)$$

where β is the level-set function of a small circle centered at the crack tip and $H(\beta)$ a smoothed Heaviside function used for mixing the different velocities on a certain predefined thickness. Dynamic anisotropic mesh adaptation is performed also to maintain the proper computation of the singular fields at the crack tip.

Crack propagation begins horizontally after 2.9s of cooling time. Figure 4 describes the temperature field after 2s.

Figure 5 illustrates the convection velocity before crack propagation at $t=2s$ and at the beginning of the propagation at $t=3s$ in a zoom near the crack tip.

It can be noticed that when $G < G_c$, $\mathbf{v}_{convec} = \mathbf{v}$ and when crack propagation begins \mathbf{v}_{convec} becomes a mixture between \mathbf{v} and \mathbf{v}_{ct} near the crack tip. It is noticed as well that \mathbf{v}_{ct} is more important than the velocity issued from the thermo-mechanical problem.

Furthermore, figure 6 shows the SLiM-Cut process at the time instants 10 and 40 seconds along with the corresponding anisotropic meshes.

It is illustrated how the crack propagated along with the opening of its faces which is insured by \mathbf{v} . Moreover, the mesh is well adapted where desired throughout the simulation.

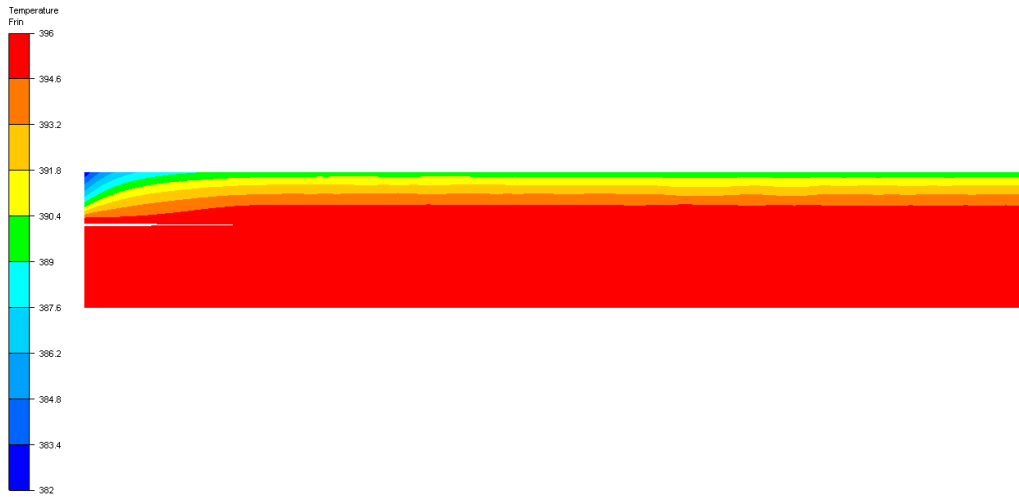


Fig. 4 – The temperature field at t=2s

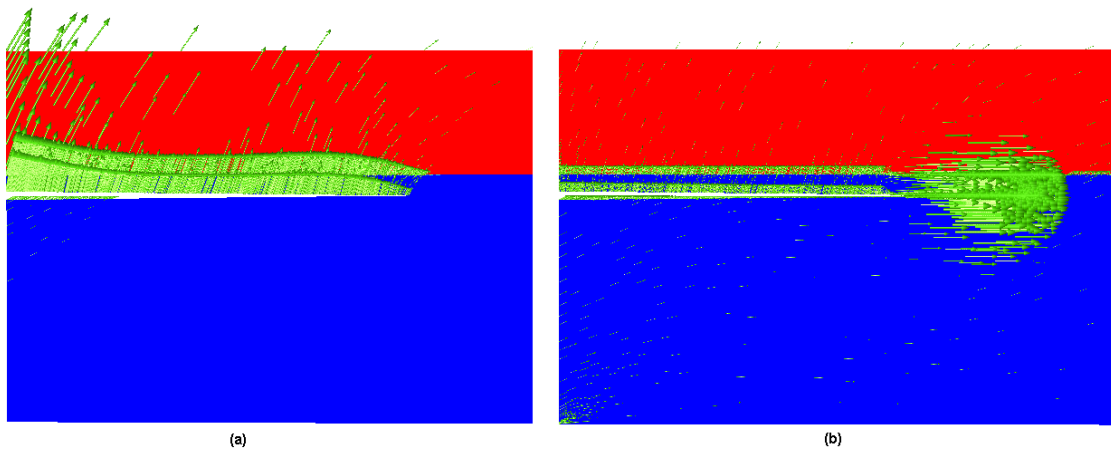


Fig. 5 – (a) $v_{convect}$ at t=2s and (b) $v_{convect}$ at t=3s

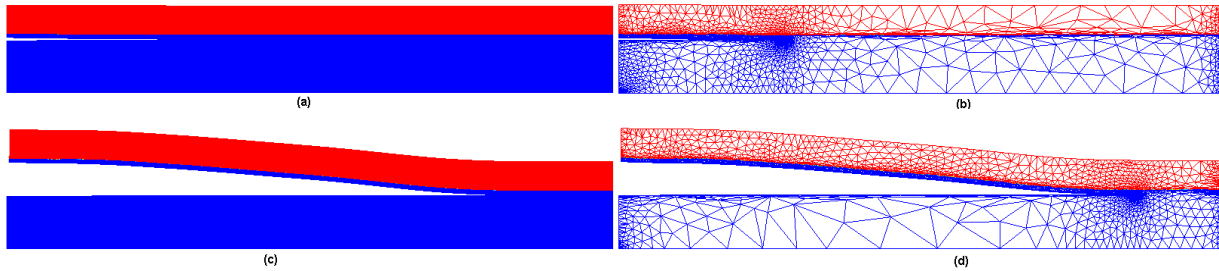


Fig. 6 – (a) The SLiM-Cut process at t=10s, with (b) the corresponding anisotropic mesh, (c) the SLiM-Cut process at t=40s, with (d) the corresponding anisotropic mesh

4 Conclusion

A monolithic method with a Lagrangian approach was introduced to model crack propagation in silicon during the SLiM-Cut process. This process is based on the idea of propagating a crack all along the interface between a stress-inducing layer and the silicon substrate in the goal of extracting a thin layer. The propagation occurs by the fact that the stress-inducing layer, having a higher thermal expansion coefficient than the silicon's, is deposited and bonded on the silicon substrate. Our method is based on the use of level-set functions for interface description, on dynamic anisotropic mesh adaptation and on the choice of an appropriate Lagrangian convection velocity. The latter is a combination between the mechanical velocity and the speed at the crack tip obtained using the $G\theta$ method.

In the two-dimensional space, our method proved its efficiency to model properly the propagation of

the crack in the mono-silicon. Extending it to the three-dimensional one, is our most important perspective.

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