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Numerical modelling and validation of thermally-induced spalling

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Abstract

In order to reduce the silicon consumption in the production of crystalline silicon solar cells, the improvement of sawing techniques or the use of a kerf-less process are possible solutions. This study focuses on a particular kerf-less technique based on thermally-induced spalling of thin silicon layers joined to aluminum. Via a controlled temperature variation we demonstrate that it is possible to drive an initially sharp crack, introduced by laser, into the silicon substrate and obtain the detachment of ultra-thin silicon layers. A numerical approach based on the finite element method (FEM) and Linear Elastic Fracture Mechanics (LEFM) is herein proposed to compute the Stress Intensity Factors (SIFs) that characterize the stress field at the crack tip and predict crack propagation of an initial notch, depending on the geometry of the specimen and on the boundary conditions. We propose a parametric study to evaluate the dependence of the crack path on the following parameters: (*i*) the distance between the notch and the aluminum-silicon interface, (*ii*) the thickness of the stressor (aluminum) layer, and (*iii*) the applied load. The results for the cooling process here analyzed show that $\Delta T > 43$ K and a ratio $\lambda=0.65$ between the thickness of the stressor layer and the distance of the initial notch from the interface are suitable values to achieve a steady-state propagation in case of a ratio $\lambda_0=0.115$ between the in plane thickness of the silicon substrate and the aluminum thickness, a value typically used in applications.

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1. Introduction

Suo and Hutchinson [1] pioneered the theoretical description of spalling in the 1980s. They found that, for certain combinations of materials and geometrical parameters of the bi-layered stack, a crack can propagate through the substrate in a steady-state manner, parallel to the interface. By exploiting this theoretical result, thin kerf-less layers of brittle material, e.g. silicon, could be produced, see [2-7].

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The theoretical model in [1] is based on the hypothesis of a two-dimensional semi-infinite plane made of a brittle material with a deposited thin film. Residual stresses induced in these components by a uniform temperature variation from a stress-free reference condition are due to the thermo-elastic mismatch between the elastic properties and the thermal expansion coefficients (CTE) of the two joined materials.

Recent experimental work on the kerf-less technology [6] proposes a temporally and spatially varying temperature field to control the crack propagation. These more complex boundary conditions, along with the fact that real samples have a finite size, require the use of a numerical method to simulate crack propagation in realistic conditions and quantify the range of parameters for stable crack propagation. Here, we present the results of the numerical simulations aiming at studying the influence of the initial notch position with respect to the aluminum-silicon interface on the stability of the crack path. We also examine the effect of two different temperature profiles, a uniform one along the whole sample, and a discrete one closer to the experimentally measured, on the computed Stress Intensity Factors (SIFs). The obtained results have important implications on the control of the spalling process and will be useful to control the roughness of the delaminated thin film, which is an undesirable effect to be minimized.

1.1. Methodology and numerical approach

Suo and Hutchinson showed in [1] that the Mode I SIF, K_I, which describes the intensity of the stress field inducing crack opening at the crack tip, is a function of the tensile stress σ_0 in the stressor layer (which depends on the imposed temperature range ΔT), of the film thickness h, of the initial position of the notch from the interface, λh, of the substrate thickness, $\lambda_0 h$, of the stiffness ratio Σ, and of the moment of inertia I of the resulting bi-layered beam, see Fig.1. In order to achieve a stable crack path and produce a planar thin layer, which is essential for the production of solar cells, it is necessary to have a steady-state crack propagation, i.e., $K_{II} = 0$ and $K_I = K_{IC}$ [8], where $K_{IC,}$ is the fracture toughness of silicon. Under these conditions, the crack propagates in a collinear manner parallel to the bi-material interface.

In this work we propose a numerical simulation of the spalling process under the assumption of plane strain conditions by using the FE program FRactureANalysis Code (FRANC2D) [9]. The discretization of the continuum is performed by using eight-node isoparametric FEs. Around the crack tip, we use quarter-point singular elements to capture the stress singularity typical of a crack travelling into a homogeneous medium. Automatic mesh refinement at the crack tip is considered during crack propagation in order to avoid the presence of geometrically distorted elements.

Simulations of crack propagation, using this code, require a series of operations. For given boundary conditions and temperature field, which is specified node-wise by a pre-processor developed in Matlab by the present authors, FRANC2D solves the linear system of equations resulting from the FE discretization. For each crack-tip position, the code computes the Mode I and the Mode II SIFs at the crack-tip via the J-integral [10] or the displacement correlation technique [11] that, for the present study, provide the same numerical results. The computed SIFs are used to predict the crack growth propagation direction based on three possible fracture criteria: the maximum shear stress criterion [12], the maximum energy release rate criterion [13], and the minimum strain energy density criterion [14]. By comparing the equivalent stress-intensity factor, determined from the SIFs according to one of these criteria, and the material fracture toughness, K_{IC}, the crack propagates if and only if it exceeds K_{IC}. Then, a new crack-tip location is determined by imposing a small user-defined crack increment in the suggested crack propagation direction. Subsequently the code deletes elements along the incremental crack path, updates crack geometry, and performs automatic local re-meshing. The details on procedures for crack propagation and re-meshing schemes are described in [15].

For this analysis we use the J-integral algorithm for the computation of the stress-intensity factors and the minimum strain energy density as the criterion to determine the crack growth direction. Thus, the crack propagates in the direction where the strain energy density S, is minimum. The strain energy density is defined as

$$S = \frac{dW}{dV} r, \tag{1}$$

where $\frac{dW}{dV}$ is the elastic energy per unit volume V and r is the radial coordinate of the polar coordinate system centered in the crack-tip. The strain energy density can also be computed from SIFs as:

$$S=\frac{1}{\pi r}(a_{11}K_{\mathrm{I}}^2+a_{12}K_{\mathrm{I}}K_{\mathrm{II}}+a_{22}K_{\mathrm{II}}^2) \tag{2}$$

where the coefficients a_{11} , a_{12}, a_{22} depend on the Young modulus E and on the Poisson ratio ν. The angle θ_0 of crack propagation is obtained as:

$$\frac{\partial S}{\partial \theta}=0 \tag{3}$$

Once the crack propagation angle is determined, the propagation criterion requires that the strain-energy-density factor reaches a critical value $S(\theta)=S_{\mathrm{C}}$. The critical value S_{C} is related to the fracture toughness of silicon, K_{IC}, and, in pure Mode I ($K_{\mathrm{II}}=0$) it is given by [15]:

$$S_{\mathrm{C}}=\frac{\kappa-1}{8\mu}K_{\mathrm{IC}}^2. \tag{4}$$

where κ is the Kolosoff constant depends on ν, the Poisson ratio, and μ is the shear modulus. Basically, the S-criterion predicts that the crack propagates when the energy density in a volume element near the crack-tip reaches a critical value.

After a finite extension of the crack, the elastic problem is solved again and the procedure is repeated.

2. Results of the parametric analysis

The 2D geometry considered and the boundary conditions are schematically shown in Fig. 1(a). We choose the geometrical parameters close to the experiments described in [6]: the thickness of the silicon substrate is $\lambda_0 h$=675 μm, and the thickness of the aluminum layer is h=120 μm. The initial notch length is a_0=190 μm, and the span of the specimen is 14 mm. The relevant material parameters are chosen from the literature and are collected in Tab. 1.

Table 1. Material parameters used in the simulations.

Material parameters	Silicon	Aluminum
E	139 GPa	68 GPa
K_{IC}	0.75 MPa $m^{0.5}$	24 MPa $m^{0.5}$
ν	0.276	0.34
CTE	0.26×10^{-5} °C^{-1}	2.3×10^{-5} °C^{-1}

2.1. Preliminary considerations on the imposed temperature range required to avoid crack arrest

We investigate the influence of the crack depth, λh, and of the distribution of the imposed temperature variation, which is considered to be a key parameter to control crack propagation and avoid crack deflection and roughness, as discussed in [6]. The FE mesh with a given notch position λh is shown in Fig. 1(b). The value of the Mode I SIF, K_{I}, related to the crack opening mode, is depicted in Fig. 2(a) vs. λ.

First, we impose a ΔT=40 K from the stress-free reference temperature over the whole specimen. We find that the smallest value of K_I is achieved for λ=0.65, see Fig. 2(a). These results are very close to the analytical predictions in [6], obtained for an infinite body.

From the computed Mode I stress-intensity factors, $K_I\,(a,\Delta T)$, corresponding to a crack length a and a given temperature range ΔT, the critical temperature range leading to crack propagation, $K_I = K_{IC}$, can be computed by a proportionality relation due to the linearity of the problem, i.e., $\Delta T_c = \Delta T\, K_{IC}/K_I\,(a,\Delta T)$. An example of computation is shown in Fig. 2(b) and (c) for λ=0.65.

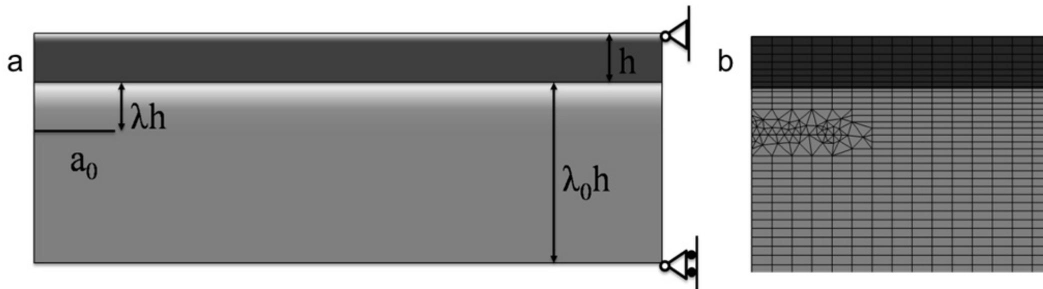

Fig. 1. (a) Geometry of the silicon substrate with an aluminum layer evaporated on the top of it, in a 2D plane strain configuration and clamped in x=14 mm; (b) zoom of the FE mesh near the crack tip, corresponding to λ=0.65

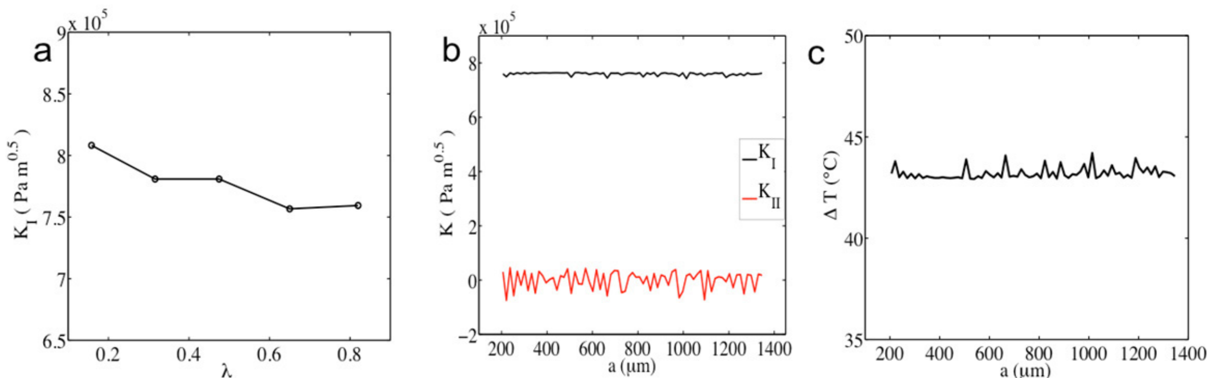

Fig. 2. (a) Influence of the crack depth λ on K_I (λ=0.158, 0.316, 0.475, 0.65 and 0.82); (b) SIFs in function of the crack length a for λ=0.65 and an uniform ΔT=40 K; (c) ΔT_c necessary to achieve crack propagation (K_I=K_{IC}).

In practical applications, a convenient way to induce spalling can be to warm up the sample from one side and then cooling it down by progressively immersing the sample in water from the opposite side, see [6]. In this case, the resulting ΔT is neither constant in time nor homogeneous over the whole body. Therefore, the steady-state crack growth cannot be analyzed with the semi-analytical model by Suo and Hutchinson [6] but needs to be investigated numerically. We analyze the effect of varying ΔT by considering ΔT_1=43 K applied to the first 1 mm of the specimen and then ΔT_2 =0 K for the rest of the specimen as shown in Fig. 3(a). We simulate the crack propagation as described before. The plot of K_I vs. the crack length a shows that in this case the Mode I stress-intensity factor is diminishing with increasing a. This is the result of a reduced fracture driving force due to a smaller ΔT at the crack tip as long as the crack moves towards the centre of the sample. When ΔT <41.7 K, then the crack arrests.

Therefore, to maintain $K_I\,(a)$=K_{IC} at the crack tip during an exfoliation experiment, a possible way is to increase the temperature range ΔT during crack propagation. Fig. 3(b) shows the temperature range from the stress-free condition that has to be applied to the first portion of the sample (geometry from Fig. 3(a)) to propagate the crack for

around 700 μm. A higher value of ΔT within the first portion of the sample is also beneficial since it leads to a larger crack opening, but the crack would eventually stop in any case in correspondence of a length $a = a^*$ when $K_I(a^*) < K_{IC}$. This behavior was also observed in the experiments [6].

Therefore, these results pinpoint that by tuning the imposed temperature range, the crack propagation can be controlled or even stopped. By limiting and localizing the area in which the exfoliation conditions are met, the formation of multiple crack fronts can be avoided, and thus surface roughness can be minimized [6].

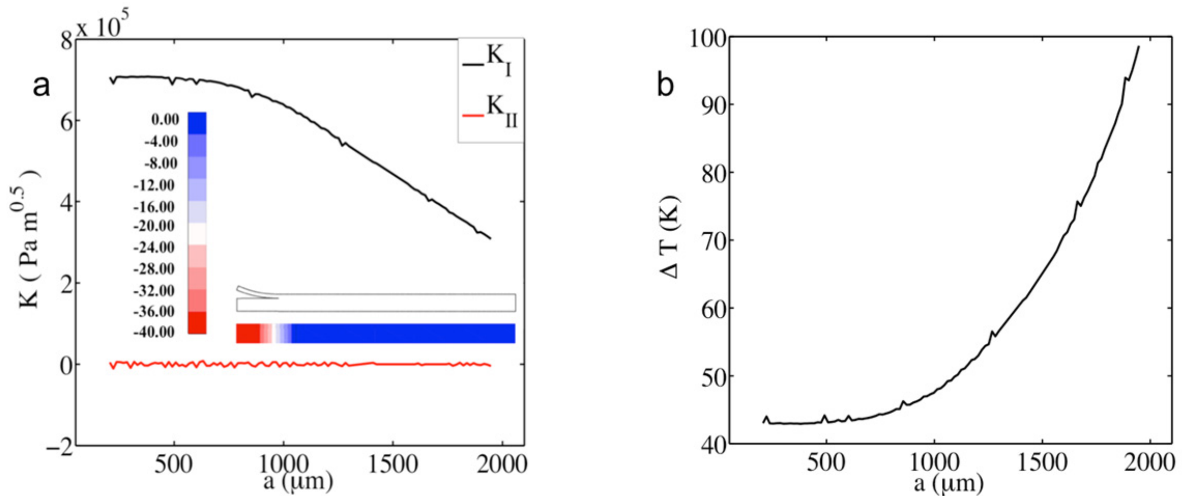

Fig. 3. (a) SIFs, deformed mesh and the discrete thermal distribution, where ΔT_1=43 K is applied for 1 mm and the other part of the sample has ΔT_2=0 K; (b) ΔT_c necessary to avoid crack arrest and propagate the crack till the end of the sample.

2.2. Parametric study and comparison with experimental results

We herein investigate the steady-state cracking position in the direction orthogonal to the aluminum-silicon interface as a function of different thicknesses of the aluminum stressor layer (*h* equal to 20, 50, 70, 100, 120, and 125 μm) and we made a comparison with our own experimental results. For the following simulations we use the thermal load resulting from the simulated thermal distribution obtained by solving the problem of heat transfer in Comsol [6] corresponding to a time of 2 s after the immersion of the sample in the water.

The resulting steady-state cracking depth λ as a function of the film substrate thickness ratio λ_0 is compared with the experimental results for *h*=40, 80, and 120 μm. The corresponding values of the thickness of the exfoliated bi-layered thin films for the three different aluminum thicknesses are 32.3±3.6 μm, 59.7±6.2 μm, and 77.4±7.7 μm. The simulation results are in accordance with the ones presented in [6] and in the case of 80 and 120 μm there is a good agree between simulated results and measured ones as shown in Fig. 4.

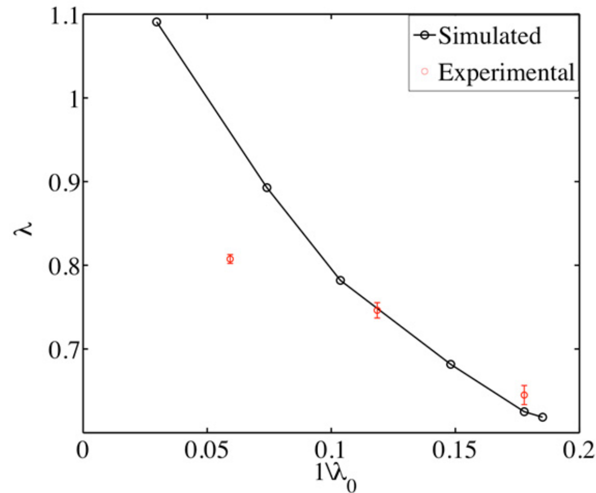

Fig. 4. Comparison between the steady-state cracking depth as a function of film substrate thickness ratio and the experimental results (in red) for *h*=40, 80, 120 μm.

Finally we investigate the influence of the anisotropy of the silicon crystal, using the same aluminum thickness (120 μm) and the thermal distribution corresponding to t=2 s after the immersion of the sample in the water bath. Experiments and simulation were carried out with two different angles of immersion (and crack propagation) with respect to the <110> lattice plane of the Si-wafer: 45° (standard orientation, (100)-direction) and 90° ((110)-direction). The thermo-elastic parameters of silicon depending on the crystal orientation are listed in Tab. 2.

Table 2. Material parameters used in the simulations for two different crystal orientations.

Material Parameters	Silicon <100>	Silicon <110>
E	139 GPa	169 GPa
K_{IC}	0.75 MPa $m^{0.5}$	0.71 MPa $m^{0.5}$
ν	0.276	0.362
CTE	$0.26x10^{-5}$ °C^{-1}	0.26 $x10^{-5}$ °C^{-1}

The computed values of K_I for the two different angles of immersion are shown in Fig.4. For the standard orientation (<100> direction), shown by the dotted blue lines, K_I outbalances K_{IC} but is lower than for the other immersion angle corresponding to the <110> direction.

The results of the final exfoliated layer thickness in stationary conditions are different for the two orientations. The measured exfoliated layer thicknesses are 77.4±7.7 μm in <100> direction and 65.1±10.2 μm in <110> direction. Both values are very close to the numerical ones: 75.91 μm for <100> and 63.64 μm for <110>.

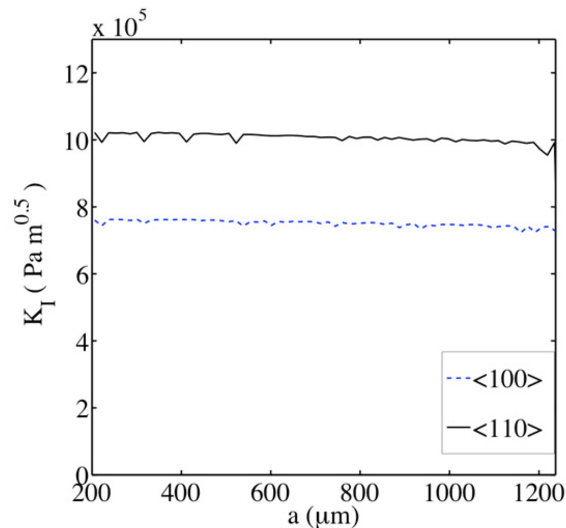

Fig. 5. Comparison between simulated SIFs for two angles of immersion respect to the <110> lattice plane of the Si-wafer: 45° (standard orientation, <100> direction, blue dotted line) and 90° (<110> direction, black line).

3. Conclusions

In the present paper, we have proposed a numerical method based on FEM and LEFM to compute SIFs and predict the crack path of an initial notch inserted by laser in an Al-Si-bilayered system. We carried out a parametric study to evaluate the dependence of the crack propagation direction on the pre-crack depth, on the applied load, on the thickness of the stressor layer and on crystal orientation of silicon with respect to the direction of immersion in water. The results show that, for the particular directional cooling process described in [6], ΔT =43 K and a stressor layer/detached layer thickness ratio of λ=0.65 and a substrate/film thickness ratio λ_0=0.115 are optimal values for achieving a steady-state crack propagation. We also validated the numerical results by comparison with experiments carried out at the Institute for Solar Energy Research Hameln (ISFH). The measurements have been compared with the results of FEM simulations showing a remarkable good agreement between the two.

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