Numerical Modelling of Thermally–Induced Spalling

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Outline

This study focuses on thermally controlled -induced spalling of thin silicon layers joined to aluminium [1] to reduce the consumption of silicon and thus of the cost.
To this aim, a numerical method based on the finite element discretization (FEM) and on Linear Elastic Fracture Mechanics (LEFM) is proposed to compute the Stress Intensity Factors (SIFs) and predict crack propagation of an initial crack, depending on geometry and on boundary conditions. A parametric study has been performed to evaluate the dependence of the crack propagation direction on the pre-crack depth, the thickness of the stressor layer and the applied load. Finally experimental data were used to validate the numerical results.

Thermally controlled-induced spalling

- Exfoliation of thin crystalline Si layer by the difference between the thermal expansion coefficient (CTE) of Si and Al-stressor layer
- Initial sharp crack introduced by laser
- Controlled thermal load propagates crack through the Si substrate ⇒ detachment of ultra-thin Si layers.

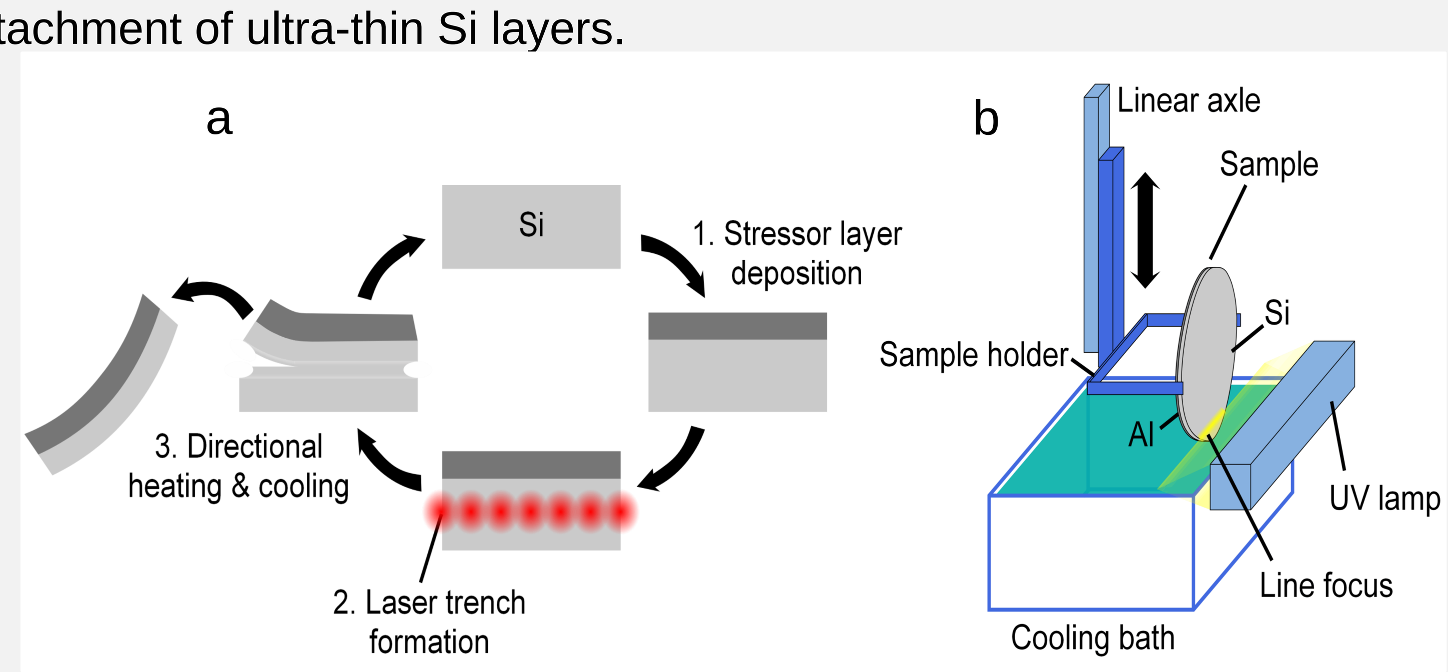

FIG. 1. (a) Process circle of exfoliation process: 1. Stressor layer deposition, 2. Laser trench formation, 3. Exfoliation by directional heating and cooling. (b) Sketch of experimental setup (not to scale): halogen-lamp (1), sample (2), sample holder (3), linear axle (4), cooling bath (5) [1].

Methodology and numerical approach

- SIFs is a function of the tensile stress σ_0 in the stressor layer (depending on ΔT), the film thickness h, the crack depth $\lambda \cdot h$, the substrate thickness $\lambda_0 . h$, the stiffness ratio **Σ** and the moment of inertia I of the resulting bi-layered system [2]
- Stable crack path and a planar thin layer ⇒ steady-state propagation $K_{II} = 0$ and $K_I > K_{IC}$ [3], where K_{IC} is the fracture toughness
- FE program FractureANalysis Code (**FRANC2D**) to compute SIFs and to predict crack propagation of the initial crack (J-integral algorithm and the minimum strain energy release rate criterion).

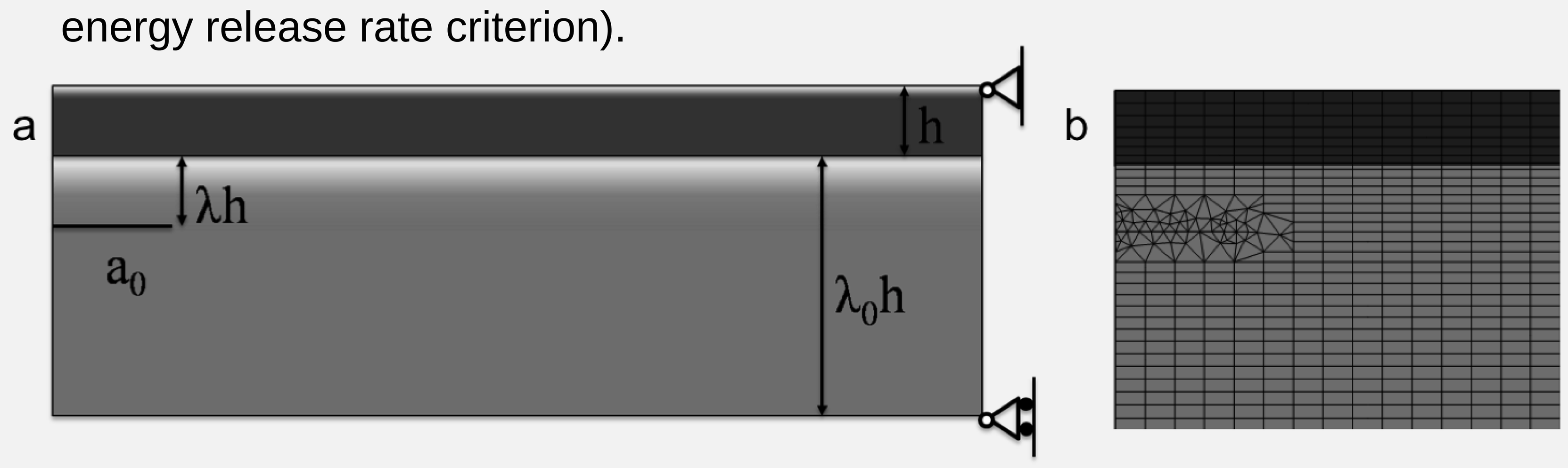

FIG. 2. (a) Geometry of the Si substrate with an Al layer evaporated on the top of it, in a 2D plane strain configuration and clamped in x=14 mm; (b) Zoom of the FE mesh, corresponding to λ=0.65.

Parametric study with uniform load

- Influence of the crack depth, $\lambda \cdot h$, on the crack propagation and crack deflection, imposing a uniform **ΔT** over the whole boundary, to achieve the steady state condition .
- The steady state value of K_I for crack propagation is achieved for **λ=0.65**, see Fig. 3 (a),very close to the analytical predictions, for the case of an infinite body, [2].

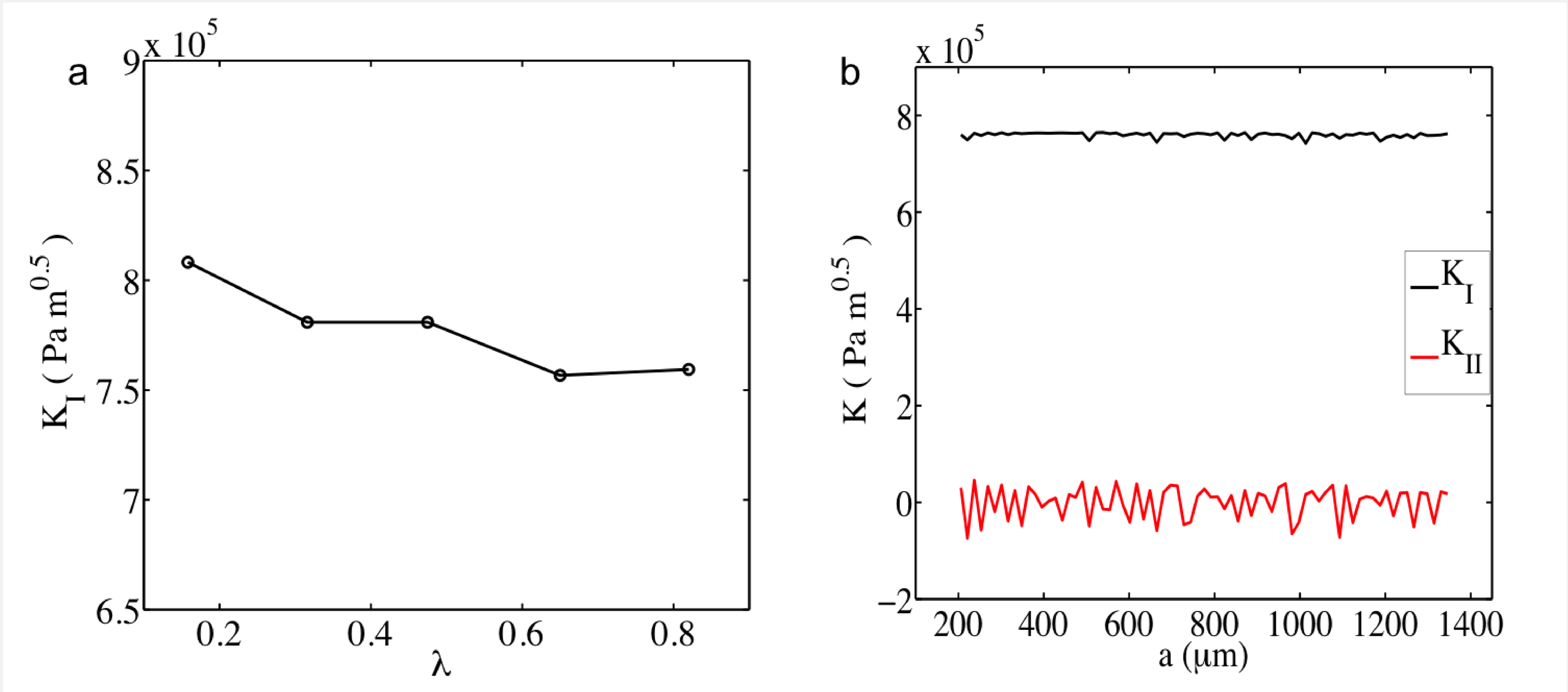

FIG. 3. (a) Influence of the crack depth λ on Mode I stress-intensity factor, K_I, related to the crack opening (simulations correspond to λ=0.158, 0.316, 0.475, 0.65 and 0.82); (b) SIFs for λ=0.65 and a uniform ΔT=40ºC.

Discrete thermal distribution

- Controlled thermal load ⇒ Discrete distribution
- ΔT_1 =43ºC applied to the first 1 mm of the specimen and ΔT_2=0ºC on the remaining sample
- Reducing of the driving force to fracture ⇒ K_I diminishes with the crack length *a*
- At ΔT =41.7ºC the crack propagation stops.

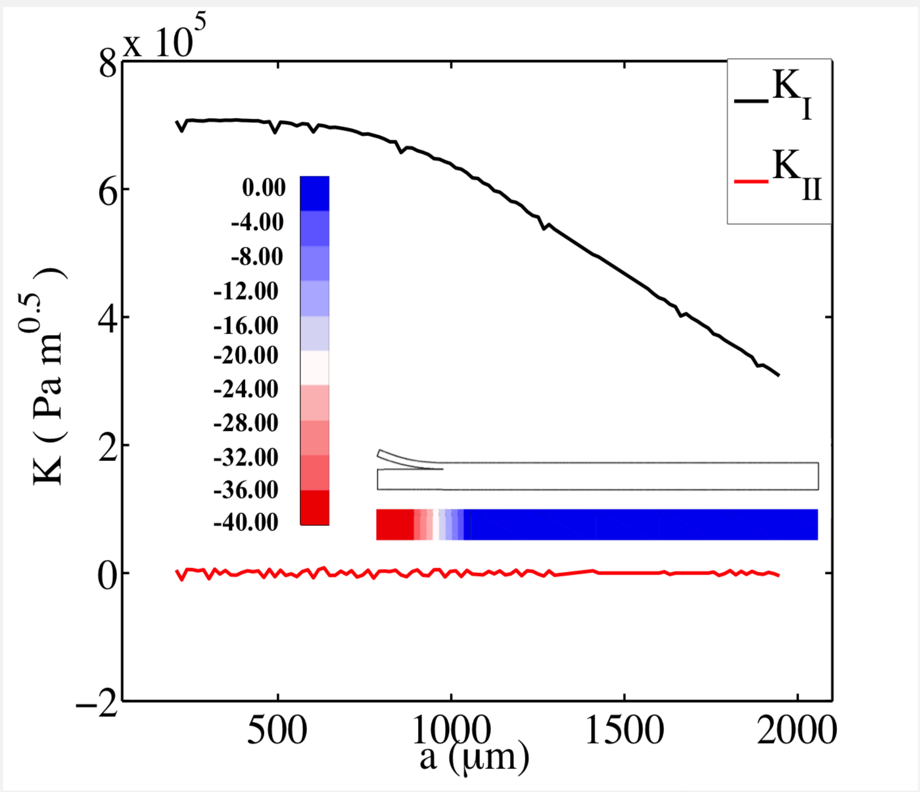

FIG. 4. SIFs, deformed mesh and the discrete thermal distribution, where ΔT_1=43ºC is applied for 1 mm and the other part of the sample has ΔT_2=0º

Validation and experimental results

Simulations:

- Different Al- thicknesses (20, 50, 70, 100, 120 and 125 μm)
- Applied load ⇒ simulated thermal distribution in Comsol in [1] corresponding to 2 s after the immersion of the sample in the water

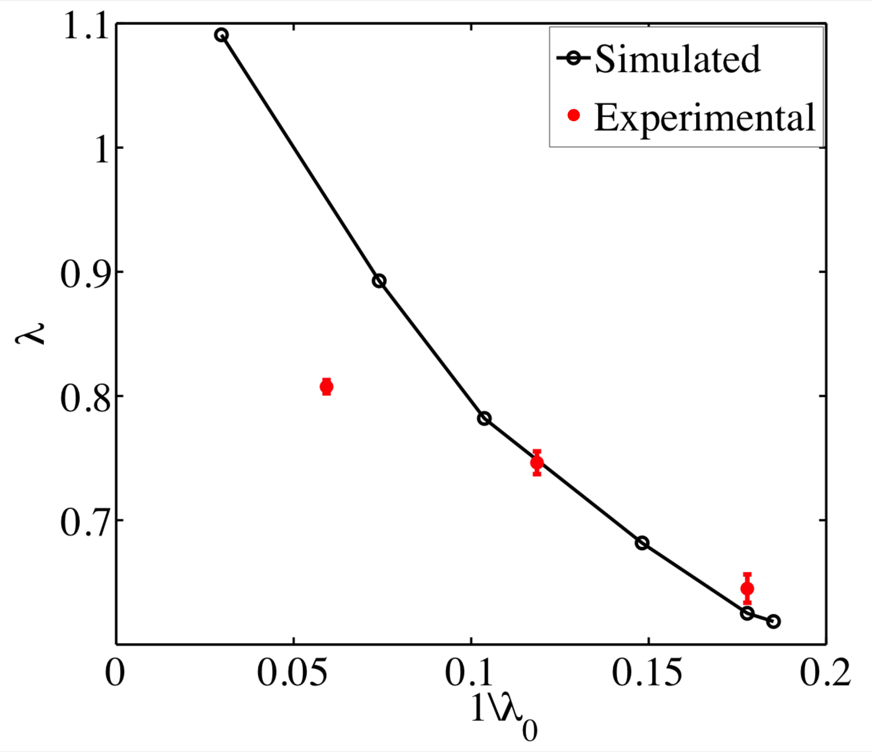

FIG. 5. Steady-state crack depth in function of film substrate thickness ratio and experimental data in red.

Table 1.

h(μm) / Exfoliated layer (μm)	40	80	120
Experimental	32.3 ±3.6	59.7±6.2	77.4±7.7

Table 2.

Orientation / Exfoliated layer (μm)	100	110
Experimental	77.4±7.7	65.1±10.2
Simulated	75.91	63.64

Simulation:

- Crystal orientation (100)-direction vs (110)-direction
- Applied load ⇒ simulated thermal distribution in Comsol in [1] corresponding to 2 s after the immersion of the sample in the water

Conclusions

- Using a numerical method based on the FEM and LEFM, we found as optimal value for steady-state crack propagation:
  - ΔT =**43ºC**
  - Ratio stressor layer/detached layer thickness ratio of **λ=0.65**
  - Ratio substrate/film thickness ratio λ_0**=0.115**
- We validated the numerical results through experimental.
- The measurements and the results of numerical simulations shown a good agreement for the thickness of the exfoliated layers.

References:

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