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Effect of interface plasticity on circular blisters

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ABSTRACT

Numerical simulations based on finite-strain elasticity and a phase-field model of dislocations reveal that dislocations are emitted at the crack-front delamination of a circular blister. It is shown that the phenomenon induces a sliding in the film-substrate interface that modifies the shape of the buckling structure. This phenomenon is theoretically quantified introducing an axisymmetric sliding into the Föppl and von-Kármán equations that describe the elastic behavior of the film. By extending the analytical investigations to the crack opening, it is shown that dislocation-induced sliding may stabilize the buckling-driven delamination of three-dimensional structures.

Delamination and buckling constitute a damage phenomenon which is frequently observed in thin film materials [1–3]. Fundamentally, buckling results from the elastic behavior of a compressed thin film as described by the Föppl and von-Kármán (FvK) model [4], which explains a wide variety of experienced morphologies (circular blisters [5], telephone cord buckles [6], etc.). At the mesoscale, the understanding of the buckling-driven delamination process is based on the concepts of fracture mechanics considering an increase of the interface toughness with the shear modes [7,8]. Although some dissipative mechanisms, such as friction [9] and plasticity [10], have already been put forward to explain a part of this mode dependence, understanding the elementary microscopic mechanisms involved during decohesion remains nowadays an important challenge.

In the last decade, several studies have been carried out to include other phenomena not considered in the aforementioned descriptions (compliant substrates [11], surface energy [12], pressure [13], etc.). The experimental observations concerning crystalline materials have also highlighted plasticity damage, like persistent folding at the base of structures, characterized subsequently by both analytical modeling and finite element simulations [14–17]. Concomitantly, atomistic simulations have been performed, notably revealing that the emission of interface dislocations modifies the shape of the straight-sided blisters [18] and affects their buckling-driven delamination [19]. A limitation of these studies is that they only consider two-dimensional situations where plasticity and fracturing are known to exhibit very different features than those observed in three-dimensional ones.

In this work, this question is addressed by investigating the effects of interface plasticity on circular blisters — the objective being to generalize such effects to more realistic three-dimensional structures. To do so, a new numerical model is used considering both cracks and individual dislocations within finite-strain elasticity formalism [20]. This letter is divided into two different parts. Simulation results showing dislocations nucleation at the crack-front of the structure and their propagation in the film-substrate interface are first reported. Then, their effects are characterized by introducing an axisymmetric sliding into the FvK equations. The results are discussed in view of the well-known features of buckling-driven delamination.

The circular blisters are simulated using a code based on finite-strain elasticity and a new phase-field model of dislocations [20]. First, we briefly recall this model considering isotropic materials.

The change in the free elastic energy is defined as:

$$\mathcal{F}_{el} = \int \frac{E}{2(1+\nu)}\left(\varepsilon_{ij}^2(\mathbf{r}) + \frac{\nu}{1-2\nu}\varepsilon_{kk}^2(\mathbf{r})\right)\mathrm{d}\mathbf{r}^3, \quad (1)$$

where E is the Young's modulus, ν is the Poisson's ratio and ε_{ij} is the Green-Lagrange strains reflecting the nonlinear geometry of the system. In this work, film, interface and substrate are considered with Young's moduli E_f, E_{int} and E_s, respectively, taken such that $E_f = 0.5\ E_s$ and $E_{int} = 0.1\ E_s$. For all of these materials, Poisson's ratio is the film's ratio, i.e. $\nu_f = 0.28$. In this model, E_{int} also controls the energy required to break the interface (toughness). In thin-film materials where blistering occurs this value is generally low, justifying the choice of 0.1 E_s [1].

Numerically, the strain/elastic field is divided into cubic elementary voxels of side d that contain the elastic information depending on whether the position $\mathbf{r}$ is related to the film, the interface or the

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substrate. These fields are computed via the displacements of the vertices of voxels which also constitute the nodes of the numerical grid. Within this framework, a crack resulting from the breaking of a given region is introduced by canceling the elastic coefficients related to the corresponding voxels. In this study, d stands for the interatomic distance but could also represent a higher length when the atomic resolution is not required.

The model also involves dislocations corresponding to the six slip-systems $\{100\}\langle 100\rangle$ of a simple cubic material. They are introduced using the eigenstrain formalism [21] combined with a phase-field description formulated at finite-strain [20]. In the present work, dislocations have the following properties: their Burgers vector norm is $b = d$, the ratio between the core energy and the elastic energy is 0.12, the core width is about 5 d, the Peierls stress is $\tilde{\sigma}_p = 0.011$ and the velocity is about $V \approx 0.06\ b\ \tilde{\tau}$ over the range of resolved shear stress $\tilde{\tau} \in [0.01, 0.05]$. Here, tildes denote stresses given in the unit of the shear modulus $\mu = E_s / (2(1 + \nu_f))$. A nucleation criterion based on the local geometry of voxels also allows the generation of dislocations at crack-front.

To simulate the circular blisters, a $200 \times 200 \times 8\ d^3$ system is built in the (x, y, z) Cartesian frame, which accounts for a thin film of thickness $h = 6\ d$ deposited on a substrate of thickness d (Fig. 1). They are separated from each other by an interface of thickness d initially free of dislocations (coherent). In the polar frame (r, θ, z), the film is delaminated from its substrate over a central circular region of diameter $r = R_0 = 50\ d$, performed by canceling the elastic coefficients of voxels constituting the interface in this region. The bottom nodes of the grid are only forced to move in their initial (r, θ) plane in order to mimic a non-compliant substrate. Free boundary conditions are set for all surfaces. Buckling is finally induced by applying a homogeneous in-plane compressive strain $\varepsilon_0 < 0$.

The purely elastic equilibrium configurations of the blister are first researched by minimizing the elastic energy of the system for different values of ε_0. In this case, expected results are obtained confirming the classical behavior of the buckling structure (Fig. 3): the blister is formed beyond a critical strain $\varepsilon_c = -0.014$ and conserves its circular shape during buckling with a maximal deflection varying as the square root of ε_0. Other results concerning the elastic behavior are also reported in Ref. [20].

Then, plasticity is allowed, switching the phase-fields on. From ε_c to $\varepsilon_0 = -0.065$, no dislocations are observed. At $\varepsilon_0 = -0.0675$, eight dislocation-loops are nucleated at the crack-front in the (001) interface plane (Fig. 2a). In the (r, θ) polar frame, the two loops around $\theta \approx 0°$ have the Burgers vector $\vec{b} = -[100]$, the two others at $\theta \approx 180°$ have $\vec{b} = [100]$, and the four loops at $\theta \approx \pm 90°$ are characterized by $\vec{b} = \mp[010]$, respectively. They occupy stable positions for the given strain, at a distance from the circular crack-front in the order of the Burgers vector. This process initiates an interface sliding mechanism of the film over the substrate. At $\varepsilon_0 = -0.07$, the previous dislocations penetrate in the interface causing the merging of the loops with identical Burgers vectors (Fig. 2b). This results in four loops occupying stable symmetrical positions in the vicinity of the crack-front. At $\varepsilon_0 = -0.08$, the previous loops overlap partially causing an inward axisymmetric displacement of about d in the interface (Fig. 2c). From $\varepsilon_0 = -0.08$ to -0.1025, the situation does not change significantly (Fig. 2d). The only change is that the four dislocation-loops penetrate further away in the interface as the compressive strain increases. They still occupy stable positions at a distance from the crack-front which roughly corresponds to the thickness of the film, i.e. $h = 6\ d$.

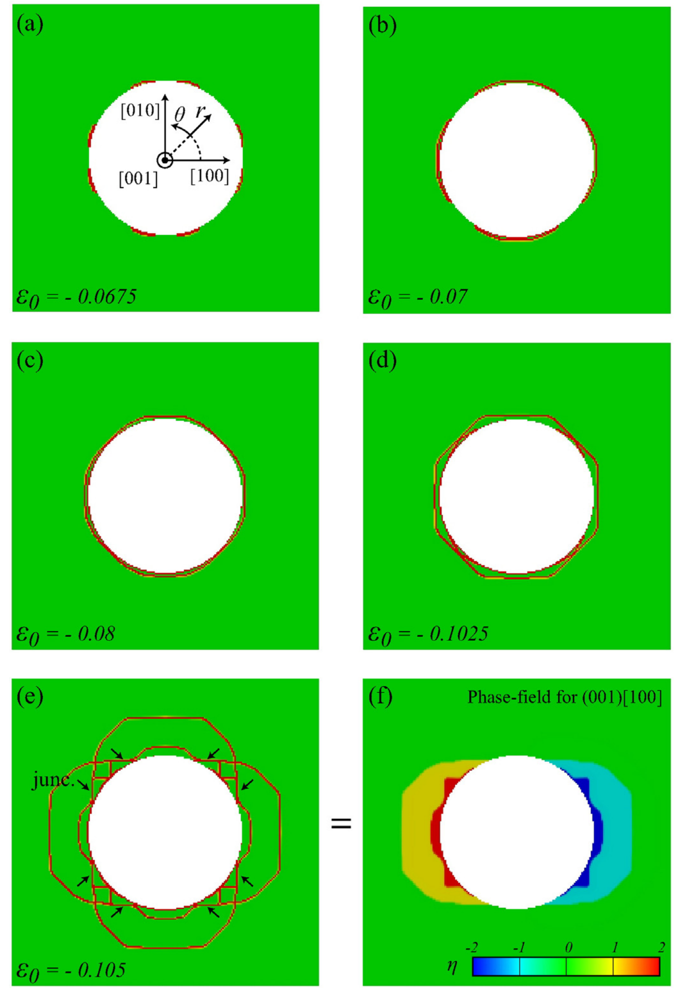

Fig. 2. Snapshots of the interface for different ε_0 revealing dislocation loops (in red) around the circular crack-front of the blister (see color online). The black arrows indicate junctions (see text). Snapshot (f) shows a mapping of (e) with respect to the phase-field parameter η related to the (001)[100] slip-system. Assuming for instance that $d = 0.5$ nm, the size of the domain is $200 \times 200\ d^2 = 100\ \text{nm}^2$.

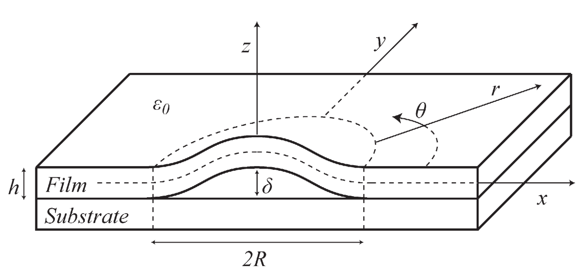

Fig. 1. Circular blister with $2R$ the diameter of the delaminated zone, δ the maximal deflection of the film, h its thickness and ε_0 the homogeneous in-plane strain.

When $\varepsilon_0 = -0.105$ is reached, four new dislocations are nucleated, identical to the first ones and spanning the same area (Fig. 2e). No equilibrium configurations are observed afterwards. To understand how the second dislocations interact with the first ones, the phase-field parameter η related to the (001)[100] slip-system is also displayed for the applied strain $\varepsilon_0 = -0.105$ (Fig. 2f). This field reflects the [100] glide along the interface plane and therefore, its discontinuities follow the dislocation line of the (001)[100] slip-system. By symmetry, the phase-field corresponding to the (001)[010] slip-system displays the same mapping, but is rotated by 90°. The analysis of Fig. 2e and f shows that these two slip-systems interact to form eight junctions (black arrows in Fig. 2e), each composed of an edge component of one slip-system and a screw component of the other. In the corresponding snapshot, film-substrate sliding consists of an inward isotropic displacement $\approx 2d$ in the interface. The simulations are finally stopped because