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3D finite element modeling for instabilities in thin films on soft substrates

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ABSTRACT

Spatial pattern formation in stiff thin films on compliant substrates is investigated based on a nonlinear 3D finite element model. Typical post-bifurcation patterns include 1D sinusoidal, checkerboard and herringbone shapes, with possible spatial modulations, boundary effects and localizations. The post-buckling behavior often leads to intricate response curves with several secondary bifurcations that were rarely studied and only in the case of periodic cells. The proposed finite element procedure allows accurately describing these bifurcation portraits by taking into account the effect of boundary conditions. It relies on the Asymptotic Numerical Method (ANM) that offers considerable advantages to get a robust path-following technique and to detect multiple bifurcations. The occurrence and evolution of sinusoidal, checkerboard and herringbone patterns will be highlighted.

1. Introduction

Surface morphological instabilities of stiff thin layers attached on soft substrates are of growing interest in a number of academic domains including micro/nano-fabrication and metrology (Bowden et al., 1998), flexible electronics (Rogers et al., 2010), mechanical and physical measurement of material properties (Howarter and Stafford, 2010), and biomedical engineering (Genzer and Groenewold, 2006) as well as biomechanics (Li et al., 2011). The pioneering work of Bowden et al. (1998) leads to several theoretical and numerical works in terms of stability study devoted to linear perturbation analysis and nonlinear buckling analysis (Huang and Suo, 2002; Chen and Hutchinson, 2004; Huang et al., 2004, 2005; Huang, 2005; Huang and Im, 2006; Im and Huang, 2008; Mahadevan and Rica, 2005; Wang et al., 2008; Song et al., 2008; Audoly and Boudaoud, 2008a,b,c; Lee et al., 2008). In most of these papers, the 2D or 3D spatial problem is discretized by either spectral method or Fast Fourier Transform (FFT) algorithm, which is fairly inexpensive but prescribes periodic boundary conditions. In this framework, several types of wrinkling modes have been observed, including sinusoidal, checkerboard, herringbone (see Fig. 1) and disordered labyrinth patterns. It has been early recognized by Chen and Hutchinson (2004) that such systems can also be studied by finite element methods, which is more computationally expensive but more flexible to describe complex geometries and more general boundary conditions, and allows using commercial computer codes. In addition, 3D finite element simulations of film/substrate instability were studied only in few papers (Chen and Hutchinson, 2004; Cai et al., 2011). Furthermore, the post-buckling evolution and mode transition of surface wrinkles in 3D film/substrate systems are rarely studied and only in the case of periodic cells (Cai et al., 2011), which still deserves further investigation, especially through finite element method that can provide the overall view and insight into the formation and evolution of wrinkle patterns in more general conditions. Can one obtain the variety of 3D wrinkling modes reported in the literature by using classical finite element models? Can one describe the whole evolution path of buckling and post-buckling of this system? Under what kind of loading and boundary conditions can each type of patterns be observed at what value of bifurcation loads? These questions will be addressed in this paper.

This study aims at applying advanced numerical methods for bifurcation analysis to typical cases of film/substrate system and focuses on the post-buckling evolution involving multiple bifurcations and symmetry-breakings, for the first time with a particular attention on the effect of boundary conditions. For this purpose, a 2D finite element (FE) model was previously developed for multiperiodic bifurcation analysis of wrinkle formation (Xu et al., submitted for publication). In this model, the film undergoing moderate deflections is described by Föppl-von Kármán nonlinear

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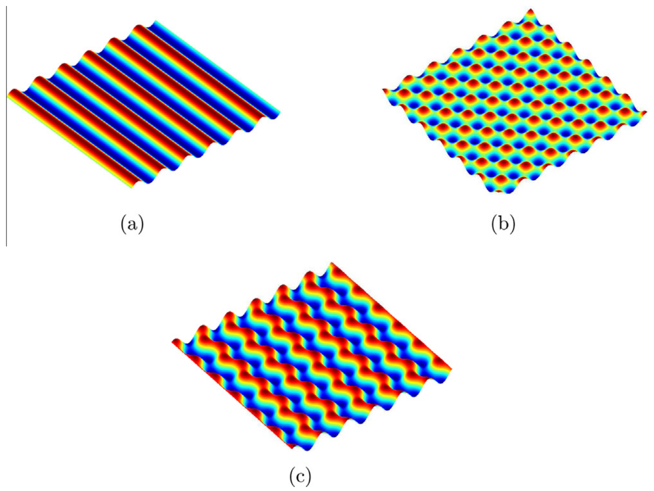

Fig. 1. Schematics of wrinkling patterns: (a) sinusoidal mode, (b) checkerboard mode, (c) herringbone mode (a periodic array of zigzag wrinkles).

elastic theory, while the substrate is considered to be a linear elastic solid. Following the same strategy, we extend the work to 3D cases by coupling shell elements to represent the film and block elements to describe the substrate. Therefore, large displacements and rotations in the film can be considered and the spatial distribution of wrinkling modes like 1D sinusoidal, checkerboard and herringbone (see Fig. 1) could be investigated.

Surface instability of stiff layers on soft materials usually involves strong geometrical nonlinearities, large rotations, large deformations, loading path dependence, multiple symmetry-breakings and other complexities, which makes the numerical resolution quite difficult. The morphological post-buckling evolution and mode shape transition beyond the critical load are incredibly complicated, especially in 3D cases, and the conventional numerical methods have difficulties in detecting all the bifurcation points and associated instability modes on their evolution paths. To solve the resulting nonlinear equations, continuation techniques give efficient numerical tools to compute these nonlinear response curves (Doedel, 1981; Allgower and Georg, 1990). In this paper, we adopted the Asymptotic Numerical Method (ANM) (Damil and Potier-Ferry, 1990, 1994; Cochelin et al., 1994, 2007) which appears as a significantly efficient continuation technique without any corrector iteration. The underlying principle of the ANM is to build up the nonlinear solution branch in the form of relatively high order truncated power series. The resulting series are then introduced into the nonlinear problem, which helps to transform it into a sequence of linear problems that can be solved numerically. In this way, one gets approximations of the solution path that are very accurate inside the radius of convergence. Since few global stiffness matrix inversions are required (only one per step), the performance in terms of computing time is quite attractive. Moreover, as a result of the local polynomial approximations of the branch within each step, the algorithm is remarkably robust and fully automatic. Furthermore, unlike incremental-iterative methods, the arc-length step size in the ANM is fully adaptive since it is determined *a posteriori* by the algorithm. A small radius of convergence and step accumulation appear around the bifurcation and imply its presence.

Detection of bifurcation points is really a challenge. Despite a lot of progresses have been made using the Newton–Raphson method, an efficient and reliable algorithm is quite difficult to be established. Indeed, it would cost considerable computing time in the bisection sequence and corrector iteration because of very small step lengths close to the bifurcation. In the ANM framework, a bifurcation indicator has been proposed to detect bifurcation points (Boutyour, 1994; Vannucci et al., 1998; Jamal et al., 2000; Boutyour et al., 2004). It is a scalar function obtained through introducing a fictitious perturbation force in the problem, which becomes zero exactly at the bifurcation point. Indeed, this indicator measures the intensity of the system response to perturbation forces. By evaluating it through an equilibrium branch, all the critical points existing on this branch and the associated bifurcation modes can be determined.

This paper explores the occurrence and post-bifurcation evolution of 1D sinusoidal, checkerboard and herringbone mode in greater depth. The paper is outlined as follows. In Section 2, a nonlinear 3D mechanical model of film/substrate system is developed. Then the resulting nonlinear problem is resolved by the ANM algorithm that is particularly efficient for computing the resulting quadratic equations and the bifurcation analysis is performed in Section 3. Results and discussion are given in Section 4, including the onset and evolution of sinusoidal wrinkles, checkerboard patterns and herringbone modes under different loading and boundary conditions. Conclusions and perspectives are reported in Section 5.

2. 3D mechanical model

We consider an elastic thin film bonded to an elastic substrate, which can buckle under compression. Upon wrinkling, the film elastically buckles to relax the compressive stress and the substrate concurrently deforms to maintain perfect bonding at the interface. In the following, the elastic potential energy of the system, is considered in the framework of Hookean elasticity. The film/substrate system is considered to be three-dimensional and the geometry is as shown in Fig. 2. Let x and y be in-plane coordinates, while z is the direction perpendicular to the mean plane of the film/substrate. The width and length of the system are denoted by L_x and L_y, respectively. The parameters h_f, h_s and h_t represent, respectively, the thickness of the film, the substrate and the total thickness of the system. Young's modulus and Poisson's ratio of the film are denoted by E_f and ν_f, while E_s and ν_s are the corresponding material properties for the substrate.

The 3D film/substrate system will be modeled in a rather classical way, the film being represented by a thin shell model to allow large rotations while the substrate being modeled by small strain elasticity. Indeed, the considered instabilities are governed by nonlinear geometric effects in the stiff material, while these effects are much smaller in the soft material. Since the originality of this paper lies in the numerical treatment of multiple bifurcations, we limit ourselves to this classical framework for the sake of consistency with previous literatures. The large rotation framework for the film has been chosen because of the efficiency of the associated finite element. Note that the same choice of a shell with finite rotations coupled with small strain elasticity in the substrate had been presented for numerical reasons in Chen and Hutchinson (2004). The application range of this model is limited by two small parameters: the aspect ratio of the film $h_f/L_x, h_f/L_y$ and the stiffness ratio E_s/E_f. In the case of a larger ratio E_s/E_f, a finite strain model should be considered in the substrate as in Hutchinson

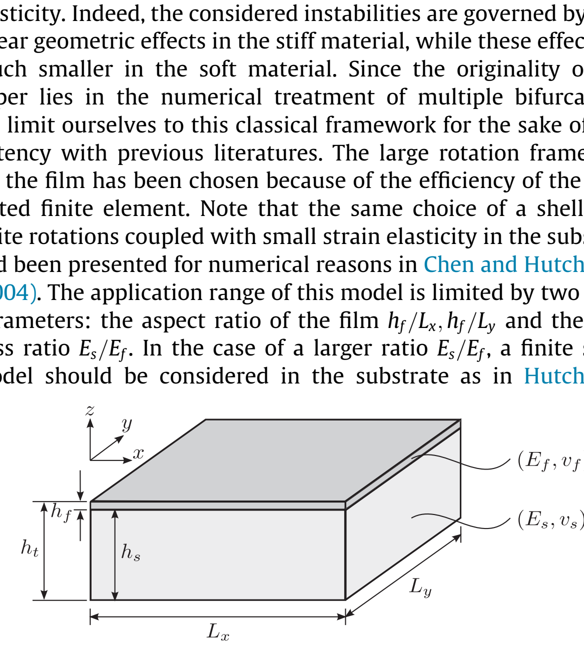

Fig. 2. Geometry of film/substrate system.