A numerical framework for pattern formation modeling of film-substrate systems

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Résumé :

Nous proposons un cadre général pour étudier le problème de flambage de systèmes film-substrat de manière numérique : de la modélisation 2D ou 3D, d'un point de vue classique ou multi-échelle. L'objectif principal est d'appliquer aux systèmes film-substrat des méthodes numériques avancées (des techniques de cheminement, des indicateurs de bifurcation, des méthodes de couplage de modèle, des analyses multi-échelle, etc.) pour des analyses de bifurcations multiples. En intégrant ces méthodes numériques avec la méthode des éléments finis, il peut prédire l'événement et l'évolution de post-bifurcation des modes d'instabilité dans diverses conditions aux limites et de chargements ainsi que les configurations géométriques complexes.

Abstract :

We propose a whole numerical framework to study the buckling problems of film-substrate systems: from 2D to 3D modeling, from classical to multi-scale perspective. The main objective is to apply advanced numerical methods (path-following techniques, bifurcation indicators, bridging techniques, multi-scale analyses, etc.) for multiple-bifurcation analyses of film-substrate buckling problems. Through incorporating these numerical methods with FEM, it can predict the occurrence and post-bifurcation evolution of wrinkling patterns in various boundary and loading conditions as well as complex geometry configurations.

Mots clefs : Wrinkling; Post-buckling; Bifurcation; Film-substrate; Path-following technique; FEM.

1 Introduction

Surface morphological instabilities of a stiff thin layer attached on a soft substrate have been widely observed in nature such as wrinkles of hornbeam leaf and human skin, and these phenomena have raised considerable research interests over the last decade [1, 2, 3]. Besides, in modern industry, surface wrinkles can be widely applied ranging from micro/nano-fabrication of flexible electronic devices with controlled morphological patterns [4, 5] to the mechanical property measurement of material characteristics [6]. In terms of stability study, several theoretical and numerical works have been devoted to linear perturbation analysis and nonlinear buckling analysis [4, 7, 8]. However, most previous works have been mainly constrained to determine the critical conditions of instability and the corresponding wrinkling patterns near the instability threshold. The post-buckling evolution and mode transition of surface wrinkles are only recently being pursued [9, 10, 11, 12].

Pattern formation modeling and post-buckling analysis deserve new numerical investigations, especially through finite element method that can provide the overall view and insight into the formation and evolution of wrinkle patterns in any condition. Therefore, we propose a whole numerical framework to study surface wrinkling of film-substrate systems: from 2D to 3D modeling, from classical to multi-scale perspective [13, 14, 15, 16, 17]. The main objective is to apply advanced numerical methods for multiple-bifurcation analyses of film-substrate systems, especially focusing on the tracing of post-buckling evolution and surface mode transition. These advanced numerical approaches include path-following techniques, bifurcation indicators, bridging techniques, multi-scale analyses, *etc.* Through incorporating them with finite element method, it can predict the occurrence and whole evolution of wrinkling patterns in various boundary and loading conditions as well as complex geometries. The point of this framework lies in, but is not limited to, the application and improvement of the following numerical methods to the instability pattern formation of film-substrate systems:

- Finite element method to be able to deal with all the geometries, behaviors and boundary conditions;

- Path-following technique for nonlinear problem resolution and post-buckling tracing;

- Bifurcation indicator to detect bifurcation points and the associated instability modes;

- Reduction techniques of models by multi-scale approaches;

- Bridging techniques to couple full models and reduced-order models concurrently.

Within this framework, both 2D and 3D models incorporate Asymptotic Numerical Method (ANM) [18, 19] as a robust path-following technique and bifurcation indicators well adapted to the ANM, so as to predict a sequence of multiple bifurcations and the associated instability modes on their post-buckling evolution path as the load is increased. The tracing of post-bifurcation response is an important and difficult numerical problem. The ANM gives interactive access to semi-analytical equilibrium branches, which offers considerable advantage of reliability compared with classical iterative algorithms. 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. Moreover, by taking the advantage 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 (see Fig. 1). To our best knowledge, it appears to be the first time that addresses the post-bifurcation instability problems of film-substrate from the quantitative standpoint, through applying these advanced numerical approaches.

Typical 3D post-bifurcation patterns include sinusoidal, checkerboard and herringbone shapes (see Fig. 2), 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 in the literature and only in the case of periodic unit cell [20]. In conventional finite element analysis, the post-buckling simulation may suffer from the convergence issue if the film is much stiffer than the substrate. However, the proposed advanced finite element procedure allows accurately describing these bifurcation portraits by taking into account the effect of boundary conditions and localizations, without any convergent problem. The occurrence and evolution of sinusoidal, checkerboard and herringbone patterns (see Fig. 2) as well as period-doubling mode (see Fig. 1) will be highlighted. The results are expected to provide insight into the formation and evolution of wrinkle patterns in film-substrate systems and be helpful to control the surface morphology, which could be used to guide the design of film-substrate systems to achieve desired wrinkling patterns for micro/nano-fabrication [21].
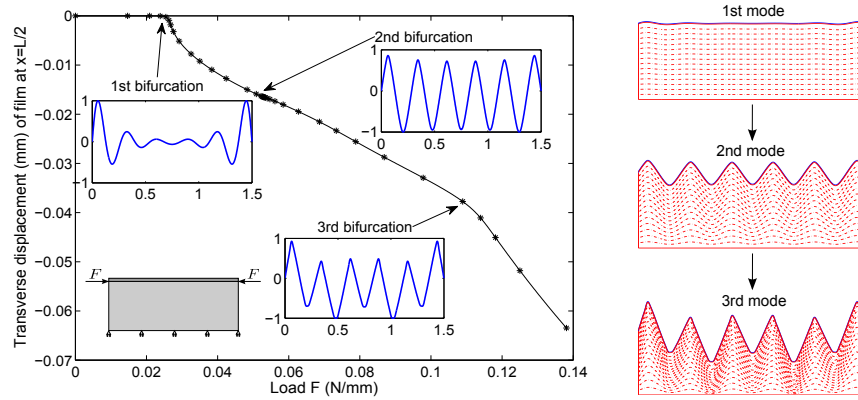
Acknowledgement

Figure 1: Bifurcation curve and the associated wrinkling modes with respect to the incremental compression. Period-doubling mode appears at the third bifurcation point.
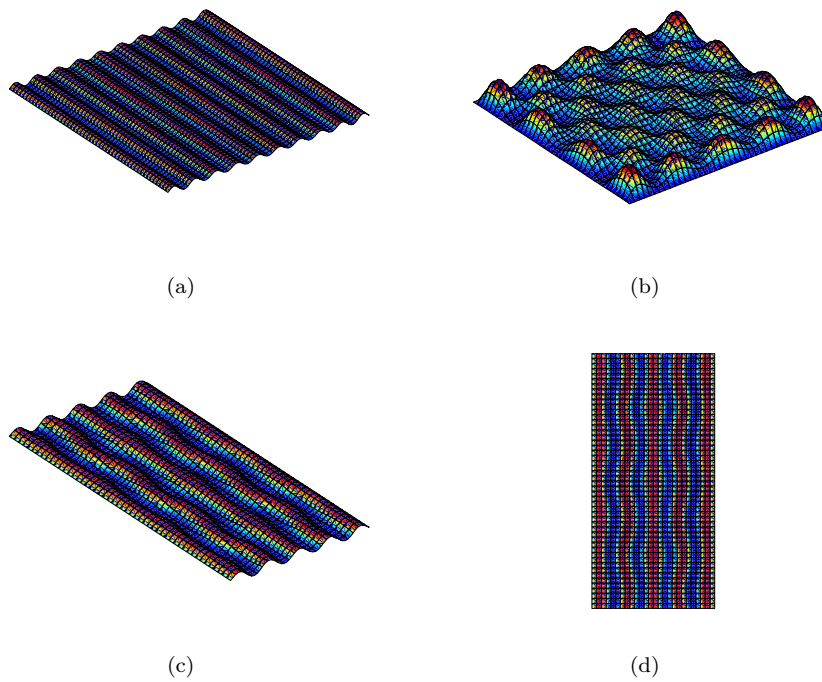

Figure 2: Numerical results on different types of 3D wrinkling patterns: (a) sinusoidal mode, (b) checkerboard mode, (c) herringbone mode, (d) top view of (c).

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