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A multi-scale modeling framework for instabilities of film/substrate systems

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ABSTRACT

Spatial pattern formation in stiff thin films on soft substrates is investigated from a multi-scale point of view based on a technique of slowly varying Fourier coefficients. A general macroscopic modeling framework is developed and then a simplified macroscopic model is derived. The model incorporates Asymptotic Numerical Method (ANM) as a robust path-following technique to trace the post-buckling evolution path and to predict secondary bifurcations. The proposed multi-scale finite element framework allows sinusoidal and square checkerboard patterns as well as their bifurcation portraits to be described from a quantitative standpoint. Moreover, it provides an efficient way to compute large-scale instability problems with a significant reduction of computational cost compared to full models.

1. Introduction

In nature, surface morphological instabilities of a stiff thin layer attached on a soft substrate have been widely observed such as wrinkles of hornbeam leaf and human skin, and these phenomena have raised considerable research interests over the last decade (Efimenko et al., 2005; Mahadevan and Rica, 2005; Stoop et al., 2015). In modern industry, surface wrinkles can be widely applied in large area ranging from the micro/nano-fabrication of flexible electronic devices with controlled morphological patterns (Bowden et al., 1998; Rogers et al., 2010), the design of coated materials or living tissues (Brau et al., 2011), to the mechanical property measurement of material characteristics (Howarter and Stafford, 2010). Several theoretical, numerical and experimental works have been devoted to stability analyses in order to determine the critical conditions of instability and the corresponding wrinkling patterns (Audoly and Boudaoud, 2008a,b,c;Chen and Hutchinson, 2004; Huang and Im, 2006; Huang et al., 2005; Song et al., 2008). In particular, there are several analytical solutions of models linearized from homogeneous finite deformation, in the case of half-spaces (Dowaikh and Ogden, 1990; Hayes and Rivlin, 1961; Shield et al., 1994) and film/substrate systems (Cai and Fu, 1999, 2000; Steigmann and Ogden, 1997). During post-buckling, the amplitude and wavelength of wrinkles will vary with respect to externally applied compressive load. Due to its well-known difficulty, most recent post-buckling analyses have recourse to numerical approaches since only a limited number of exact analytical solutions can be obtained in very simple or simplified cases. In most of early numerical studies,

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the 2D or 3D spatial problem of film/substrate is often discretized by either spectral method or Fast Fourier Transform (FFT) algorithm, which is fairly computationally inexpensive but prescribes periodic boundary conditions and simple geometries. Recent efforts have been devoted to 2D or 3D numerical study of film/substrate buckling by using finite element method (Cai et al., 2011;Cao and Hutchinson, 2012a,b;Cao et al., 2012; Stoop et al., 2015; Sun et al., 2012; Xu et al., 2014b, 2015a,b; Zang et al., 2012), which is more computationally expensive but more flexible to describe complex geometries and general boundary conditions, and also allows using commercial computer codes.

The previous works of Xu (2014) and Xu et al. (2014a,b, 2015a,b) proposed a whole numerical framework to study surface wrinkling of thin films bound to compliant substrates, through applying advanced numerical methods for bifurcation analyses and focusing on the post-buckling evolution involving multiple bifurcations, which for the first time addressed the post-bifurcation response of film/substrate systems from a quantitative standpoint. In this framework, the emergence and post-buckling evolution of several typical 2D or 3D wrinkling modes like sinusoidal, period-doubling, checkerboard and herringbone were thoroughly investigated (Xu et al., 2014b, 2015a,b). In addition, the effects of a large range of stiffness ratio E_f/E_s from $O(1)$ to $O(10^5)$ on instability patterns and the choices of different modeling frameworks, i.e. small strain linear elasticity or finite strain hyperelasticity, were deeply discussed. In these cases, the spatial shape of system responses looks like a slowly modulated oscillation and direct simulation of such cellular instabilities in a big sample often requires numerous degrees of freedom. Therefore, from the computational point of view, it would be interesting and important to develop reduced-order models to dramatically cut the computational cost and time, and to be able to simulate a large number of wrinkles.

A multi-scale approach based on the concept of Fourier series with slowly varying coefficients has been developed to study the instabilities with nearly periodic patterns (Damil and Potier-Ferry, 2006, 2008, 2010). It has been successively applied to the buckling of a long beam lying on a nonlinear elastic foundation (Mhada et al., 2012; Xu et al., 2014a), global and local instability interaction of sandwich structures (Liu et al., 2012; Mhada et al., 2013), and membrane wrinkling (Damil et al., 2013, 2014). This multi-scale approach is based on the Ginzburg–Landau theory (Iooss et al., 1989; Wesfreid and Zaleski, 1984). In the proposed theory, the envelope equation is derived from a double-scale analysis and the nearly periodic fields (reduced-order models) are represented by Fourier series with slowly varying coefficients. This mathematical representation yields macroscopic models in the form of generalized continua. In this technique, the macroscopic field is defined by Fourier coefficients of the microscopic field. It has been established that the models obtained in this way are consistent with the Ginzburg–Landau technique, but can remain valid away from the bifurcation (Damil and Potier-Ferry, 2010).

This work aims at building a multi-scale reduced modeling framework based on this Fourier-related technique to study the occurrence and evolution of film/substrate instability phenomena. A general macroscopic modeling framework will be derived first, which can be directly used for any 3D film/substrate discretization at the expense of computational cost and flexibility. Then a simplified 3D macroscopic model will be proposed by taking into account the property of film thinness, through associating a nonlinear macroscopic plate model representing the film and a linear macroscopic elasticity describing the substrate. The model incorporates Asymptotic Numerical Method (ANM) (Cochelin, 1994; Cochelin et al., 1994, 2007; Damil and Potier-Ferry, 1990) as a robust path-following technique to predict secondary bifurcations on their post-buckling evolution path as the load is increased. The tracing of post-bifurcation response is an important but difficult numerical problem. The ANM gives interactive access to semi-analytical equilibrium branches, which offers considerable advantage of reliability compared to classical iterative algorithms. By taking 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 a bifurcation point and imply its presence.

This paper investigates the appearance and post-buckling evolution of instability patterns of 3D film/substrate systems, for the first time starting from a multi-scale standpoint. The paper is organized as follows. In Section 2, a generalized macroscopic modeling framework is presented first. Then in Section 3, a simplified 3D macroscopic model is derived, which couples a nonlinear macroscopic plate model to represent the film and a macroscopic linear elastic solid to describe the substrate. The resulting nonlinear problem is then reformulated by the ANM algorithm as a path-following technique in Section 4. Results and discussions are provided in Section 5, including the onset and evolution of sinusoidal wrinkles, square checkerboard patterns and alternating packets of large and small amplitude undulations. Conclusions and perspectives are reported in Section 6.

2. General macroscopic modeling framework

We will conduct a multi-scale approach based on the concept of Fourier series with slowly varying coefficients. Let us suppose that the instability wave number q is known. In this way, all the unknowns of model $U(x) = \{u(x), s(x), \gamma(x), \ldots\}$ can be written in the form of Fourier series, whose coefficients vary more slowly than the harmonics:

$$U(x) = \sum_{j=-\infty}^{+\infty} U_j(x)e^{jiqx}, \tag{1}$$