Deformation Instabilities of Thin Films on a Compliant Substrate: Direct Numerical Simulations

Siavash Nikravesh, Yu-Lin Shen Department of Mechanical Engineering University of New Mexico

Donghyeon Ryu

Department of Mechanical Engineering New Mexico Institute of Mining and Technology

Abstract

Formation of instabilities is commonly encountered in thin film-substrate systems subjected to thermo-mechanical compressive loading. In this paper, our recent development on a practical finite element modeling approach to predict the wrinkling/buckling instabilities is presented. The numerical technique is based on the incorporation of embedded imperfections in the model. Examples of the numerical results and directions for future studies are also briefly discussed.

Introduction

Surface instability of film/substrate systems is a commonly observed feature in devices such as flexible electronics and optoelectronics. Instability-driven undulations, while frequently undesirable, has been increasingly exploited to enhance device performance; controlling wrinkle formation is thus of great importance, which calls for robust design tools. Numerical simulation of such instability problems has always been challenging. The common approach frequently reported in the literature¹ consists of laborious two-step pre-buckling and post-buckling analyses: a linear modal analysis is performed in the pre-buckling step, and a combination of nonlinear material model and geometric imperfections (with aspect ratios corresponding to the critical mode-shape found in the pre-buckling step) is then carried out in the post-buckling analysis. The implementation is tedious and the results are highly sensitive to the shape/distribution of the simulations of surface instability in single-layer film systems; the applicability and reliability to the multi-layer film/substrate systems as well as the possible development of global instability have not been proven. Here, our recent development on a practical finite element modeling approach to predict the film-substrate instabilities is presented.

Numerical Technique Overview

With the numerical technique recently proposed by Nikravesh et al.^{2,3}, the film/substrate instabilities were successfully simulated by incorporation of "embedded imperfections" (elements with perturbed material properties) immediately underneath the film/substrate interface. It was observed

Proceedings of the 2020 ASEE Gulf-Southwest Annual Conference University of New Mexico, Albuquerque Copyright © 2020, American Society for Engineering Education that placement of such material defects not only initiates deformation instability but also leads to direct evolution of such instability in a seamless manner. Large-scale planar finite element simulations were conducted considering single-layer or multilayer thin films on a very thick compliant substrate under displacement-controlled compression. The constitutive model used for the simulations were linear elastic coupled with geometric nonlinearity. The temporal evolution of the wrinkling wavelength and amplitude, as well as the critical strain to activate the instability, were all predicted in a straightforward manner. The results were verified with available analytical solutions. The effects of imperfection distribution and material properties were systematically studied^{2,3}. An example of the simulated surface wrinkles is shown in Figure 1a. With a reduced substrate thickness, global buckling of the film/substrate structure can also be directly simulated (Figure 1b). This numerical approach is not limited to 2D simulations; it can be readily implemented in 3D film/substrate models. As an example, a representative result of uniaxial wrinkling mode from a 3D simulation is shown in Figure 1c. The same approach may also be applied to cases involving nonlinear film/substrate systems with various plasticity, damage, and delamination models.



Figure 1. Representative numerical results of deformed configurations associated with (a) surface wrinkling (b) global buckling, and (c) 3D simulation of uniaxial wrinkling.

Summary and Conclusions

Our current numerical approach based on embedded imperfections is able to directly simulate wrinkling and buckling instabilities displayed by the thin film-thick compliant substrate structures. The technique is robust, easy to implement, and it overcomes the challenges in computationally modeling film-substrate instabilities. The current approach enables increased accuracy and versatility in predicting instabilities over a wide range of material and geometric conditions.

References

- 1 Huck, W. T. *et al.* Ordering of spontaneously formed buckles on planar surfaces. *Langmuir* **16**, 3497-3501 (2000).
- 2 Nikravesh, S., Ryu, D., Shen, Y.-L. Direct numerical simulation of buckling instability of thin films on a compliant substrate. *Advances in Mechanical Engineering* **11**, 1687814019840470, doi:10.1177/1687814019840470 (2019).
- 3 Nikravesh, S., Ryu, D., Shen, Y.-L. Surface Instability of Composite Thin Films on Compliant Substrates: Direct Simulation Approach. *Frontiers in Materials* **6**, 214 (2019).

Proceedings of the 2020 ASEE Gulf-Southwest Annual Conference University of New Mexico, Albuquerque Copyright © 2020, American Society for Engineering Education