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# A multi-scale simulation of tungsten film delamination from silicon substrate

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**Abstract**

To bridge the different spatial scales involved in the process of tungsten (W) film delaminating from silicon (Si) substrate, a multi-scale simulation procedure is proposed via a sequential approach. In the proposed procedure, a bifurcation-based decohesion model, which represents the link between molecular and continuum scales, is first formulated within the framework of continuum mechanics. Molecular dynamics (MD) simulation of a single crystal W block under tension is conducted to investigate the effect of specimen size and loading rate on the material properties. The proposed decohesion model is then calibrated by using MD simulation of a single crystal W block under tension and using available experimental data, with a power scaling law to account for the size effect. A multi-scale model-based simulation of W film delamination from Si substrate is performed by using the proposed procedure within the framework of the material point method. The simulated results provide new insights into the mechanisms of the film delamination process.


*Keywords:* Multi-scale simulation; Film delamination; Molecular dynamics; Size effect

## 1. Introduction

Thin films usually develop high residual stresses during the deposition process. The films subjected to large residual stresses may fail by delaminating and buckling away from the substrates in the working environment. The delamination of compressed films has been studied by many researchers in both academia and industry, as shown by representative papers (Gioia and Ortiz, 1997; Hutchinson and Suo, 1991;

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Wan and Mai, 1995). Existing approaches are mainly based on conventional elastic stability theory and interfacial fracture mechanics, with a focus on the stability of blisters (Audoly, 1999). Recently, much research has been conducted to model and simulate pattern formation during the delamination process, based on the buckling-driven mechanism (Crosby and Bradley, 1999; Huang and Suo, 2002; Moldovan and Golubovic, 1999; among others). However, a systematic study of the complete process from the formation of films to their eventual delamination from substrates is not yet available from the open literature, due to the complexity of multi-physics and multi-scales involved.

Based on the experimental observation of the transition from tensile to compressive stress as a function of the argon gas pressure in magnetron sputter-deposited tungsten (W) film onto silicon (Si) substrate (Shen et al., 2000), Chen et al. (in press) proposed that the delamination of compressed films is essentially due to the interaction between geometrical and material instabilities which results in the formation and evolution of localization, depending on different stress states in the domain of influence. By formulating a bifurcation-based decohesion model within the framework of the material point method (MPM), which is one of the "meshfree" methods (Chen et al., 2002), a numerical effort was made to investigate the transition from continuous to discontinuous failure modes involved in the W film delaminating from the Si substrate. Within the framework of continuum mechanics, the numerical study of the effects of aspect ratio and failure mode on the evolution of failure patterns under different boundary conditions provides a better understanding on the physics behind the film delamination process (Chen et al., in press).

However, the bifurcation-based simulation of the transition from localization to decohesion in the film delamination process is based on a phenomenological framework which could only provide a qualitative analysis of film delamination process. The bifurcation-based decohesion model, as proposed by Chen et al. (in press) is formulated via thermodynamics constraints with the result that the dissipation inequality is automatically satisfied. However, the constitutive relation of decohesion–traction, $\tau(\bar{u})$, as a key part of the decohesion model, cannot be calibrated via existing experimental techniques. Since the decohesion–traction constitutive relation is directly related to the interatomic binding energy and film microstructure developed during the film formation process, atomistic simulation might provide required information for establishing the decohesion model. Furthermore, the size of the film–substrate structure usually ranges from nano/micro to macroscale, and which is beyond the capability of the conventional continuum mechanics. Hence, a multi-scale decohesion–traction model is required to accommodate the suitable constitutive laws for the film structures at different size scales. In other words, a thorough understanding of the physics behind the film delamination process necessitates a multi-scale investigation ranging from atomistic simulation to continuum mechanics.

For the purpose of simplicity, a multi-scale sequential approach is proposed in this study, as illustrated in Fig. 1, to simulate the film delamination process. When bifurcation occurs in the MPM discretization of macroscopic responses, the proposed procedure would zoom in to the desired scale level in order to obtain the $\tau(\bar{u})$ constitutive relation curve. By coupling the multi-scale $\tau(\bar{u})$ constitutive law with the discontinuous bifurcation analysis within the framework of the MPM, the multi-degree discontinuous failure modes involved in the film delamination process could then be simulated.

With the rapid development of micro-electromechanical systems (MEMS) and nano-technology, atomistic simulation of mechanical behavior of metals has drawn considerable attention in recent years (Horstemeyer et al., 2001; Hu et al., 1998; Li and Yip, 2002; Liang and Zhou, 2003; Makarov et al., 2001; among others). The deformation of atomic system at finite temperatures in general is an intrinsically dynamic process. Size and strain rate effects arise out of several factors and play important roles in determining the response of nano-structures. The behavior and properties of micro/nano-structure are size-dependent due to the discreteness of atomic system, crystal arrangement and boundary condition. The dynamic inertia effect and the finite speeds at which lattice waves propagate also introduce the size effect to the problem and contribute to the size-dependence of atomic behavior. The inertia effect and finite wave speeds, along with