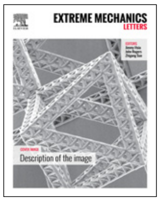
Extreme Mechanics Letters 4 (2015) 175–185

Contents lists available at ScienceDirect

Extreme Mechanics Letters

journal homepage: www.elsevier.com/locate/eml



Modelling wrinkling interactions produced by patterned defects in metal thin films

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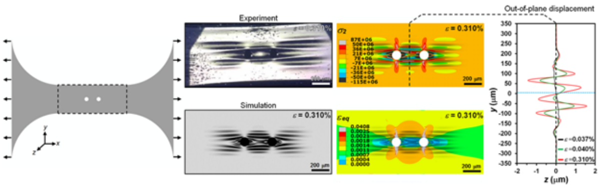
GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 22 December 2014
Received in revised form 10 June 2015
Accepted 9 July 2015
Available online 11 July 2015

Keywords:
Freestanding metal thin film
Wrinkling patterns
Patterned defects
Post-buckling analysis
Finite-element simulations

ABSTRACT

Wrinkling patterns in freestanding metal thin films under tensile loading are investigated through finite-element simulations with experimental validation. Numerical simulations of the tensile testing of a thin film specimen with different arrays of holes were conducted. Good agreement between experiments and simulations was found for not only the spatial wrinkling pattern distributions, but also the pattern evolution over the different loading stages. The numerical results show that plasticity plays an important role in the evolution of wrinkling patterns and their associated interactions in Al thin films. It was found that the spacing between defects and defect size control the level of interaction between wrinkle branches generated by the defects. Strong interactions resulted in the merging of different wrinkle branches into one single wrinkle with a large displacement amplitude and a well-defined profile in the out-of-plane direction. The simulations proved to be robust in their descriptions of the experimentally observed wrinkling phenomenon and could be used to predict wrinkling in other hole-patterned thin film configurations. The interaction and merging of wrinkle branches from multiple holes indicate that the resulting wrinkle patterns can be manipulated by using different defect configurations to achieve a desired wrinkled "microstructure".

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http://dx.doi.org/10.1016/j.eml.2015.07.002
2352-4316/

1. Introduction

Wrinkling patterns are commonly encountered in thin film structures and membranes subjected to local compressive stresses, either in loaded freestanding conditions [1,2] or via mechanical mismatches with substrates [3–7]. The pattern and its evolution can be controlled through different means of stress generation, e.g., applied lateral displacements [8,9], temperature variation [10], surface tension via liquid–solid interaction [11], and controllable residual stresses [12–15]. Specific wrinkling patterns can be designed to achieve desired functions in thin film systems, via changing surface morphology and roughness [16–18], wetting and adhesive properties [11,18], tuneable mechanical properties [19], and generating micro-fluidic channels [20]. These wrinkling patterns manifest in structural [14,21], biological [6,22], electronic (e.g., 2D materials) [23], and metrology applications [3,9], but most modelling efforts treat materials as defect-free. Defects in such 2D and layered materials are common and may control the nucleation and propagation of wrinkling patterns [24–28]. However, despite intense research efforts on the mechanical response of thin films ranging from necking instabilities to wrinkling mechanisms [29–33], all of which are crucial for thin film heterostructures and flexible electronics applications, the influence of defects within thin membranes in controlling the wrinkling patterns has not received much attention, particularly in metallic thin films.

To address this gap in current knowledge, we perform numerical simulations to model freestanding metal thin films with different types of pre-patterned defects subjected to remote uniaxial stretches with an emphasis on the development and evolution of the resulting wrinkling patterns and their interactions. We modelled intentionally-defected metallic thin films with arrays of holes to investigate how the spatial and configurational variation of the defects affects the overall wrinkling patterns and interactions of individual wrinkle branches. These numerical simulations are validated by comparing with experiments on patterned submicron Al thin films, showing that the simulations faithfully reproduced the wrinkling patterns. Our simulations use the finite element method (FEM) and have been performed with consideration of the full elastic–plastic behaviour of the material and initial residual stresses, to not only predict the evolution of complex wrinkling patterns and their interactions but also to access the stress and strain fields.

2. Methodology

Here, we consider Al thin films as typical examples of metallic films, which are commonly used in many technological applications such as in stretchable electronics [34]. Wrinkling patterns in thin metallic films have not been studied as widely as polymer membranes, with the important difference between these two classes of thin films being the occurrence of plasticity. In this letter, we will perform a full elastic–plastic numerical analysis for various geometries of patterned defects to investigate the wrinkling patterns and their interactions, with detailed experimental validation. Due to the difficulty of experiments on these films, the tensile tests were performed only on three different arrays of holes. We will focus on the additional information provided by numerical simulations and analyse the results systematically, such as the inhomogeneous stress and strain fields and the role of defect spacing, which are of critical importance for the understanding of interactions between wrinkles.

2.1. Finite-element modelling

To investigate the effect of defects on wrinkling in tensile testing of Al thin films, we constructed FEM models using the software Abaqus [35] with an implicit solver. The geometry and dimensions of the thin film model are shown in Fig. 1. The models were meshed using conventional quadrilateral shell elements (S4R) with a large-strain formulation, allowing transverse shear deformation. Although the minimum size of the shell elements is approximately 15 times larger than the film thickness, it is smaller than the typical expected wavelength of the wrinkling pattern as observed in experiments. The mesh was refined in regions near the holes, where larger changes in stresses are expected (Fig. 1(a)). A mesh sensitivity analysis showed that this level of mesh refinement was deemed sufficient for our numerical model.

To represent the pre-stressed state of these thin films before the tensile test owing to residual stresses that develop during film deposition, we applied an eigenstrain via a virtual increase of film temperature resulting in an estimated equi-biaxial compression stress on the film. This approach has been successfully used in thin film buckling analyses [15,36]. The magnitude of this equi-biaxial stress was estimated in the range between 10 and 50 MPa, which is similar in magnitude to reported values for stresses from the thermal expansion mismatch between Al and Si [37]. During the strain-release process of this biaxial compressive stress, wrinkling can initiate in the simulations. Subsequently, the edges of the film were uniaxially stretched to approximately 30 μm.

For all simulations, we employed an elastic–plastic material model, which was based on experimental stress–strain curves from tensile testing of an Al specimen without patterned holes in the gauge section [38]. It has been reported that the temporal evolution of grain size and distribution play important roles in governing the plasticity in this type of material [38]; however, we limited the scope of this work to a time-independent stress–strain curve for the material model, which was found to be sufficiently accurate for our numerical simulations. For Al films, the material model used a von Mises yield criterion with isotropic hardening. The following material properties were employed: Young's modulus $E = 70$ GPa, Poisson's ratio $\nu = 0.34$, and yield strength $\sigma_Y = 80$ MPa [38].

We performed instability calculations in our FEM model to understand the complex deformation state that arises in the thin film geometry. Thin stressed membranes are known to develop instabilities that cause the material to wrinkle out-of-plane. Buckling analyses were performed based on the Riks method [39,40] due to the nonlinearity in geometry and plastic behaviour during the tensile loading. The Riks method uses the load magnitude as an additional independent parameter and it solves simultaneously