Probabilistic Engineering Mechanics 49 (2017) 1–12

Contents lists available at ScienceDirect

Probabilistic Engineering Mechanics

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

Stochastic homogenization of nano-thickness thin films including patterned holes using structural perturbation method

Hyunseong Shin [a], Seongmin Chang [b], Joonho Jeong [c], Maenghyo Cho [d,*]

[a] Electronic Convergence Materials & Device Research Center, Korea Electronics Technology Institute, #25 Saenari-ro, Bundang-gu, Seongnam-si, Gyeonggi-do 463-816, Republic of Korea

[b] SMART Reactor Design Division, Korea Atomic Energy Research Institute, 111, Daedeok-daero 989 beon-gil, Yuseong-gu, Daejeon, 34057, Republic of Korea

[c] Research Reactor System Engineering Team, Research Reactor Development, Korea Atomic Energy Research Institute, 111, Daedeok-daero 989 beon-gil, Yuseong-gu, Daejeon, 34057, Republic of Korea

[d] Department of Mechanical & Aerospace Engineering, Seoul National University, Seoul 151-744, Republic of Korea

ARTICLE INFO

Keywords:
Stochastic multiscale analysis
Monte-Carlo simulation
Homogenization
Surface effect
Structural perturbation method

ABSTRACT

The aim of this paper is to investigate the statistical response of the homogenized mechanical behavior of nano-thickness thin films with circular holes. For this purpose, a stochastic multiscale framework is proposed. The proposed framework involves molecular dynamics simulation, surface modeling, asymptotic homogenization, moving-mesh technique, Monte-Carlo simulation, and a reduced computational scheme. The surface effect of thin-film material is predicted by the molecular dynamics (MD) approach. The volume fraction and location of each circular hole are considered as geometric uncertainties of a model. In order to investigate the statistical response of the homogenized mechanical behavior, Monte-Carlo simulation is performed to show the probability density distribution of the homogenized elastic modulus against geometric uncertainties. The reduced computational schematic based on the static reduction method and the structural perturbation method is proposed in order to overcome the issues of a cumbersome remeshing procedure and computational inefficiency of Monte-Carlo simulations involving a high number of repetitive trials. A guideline to minimize the coefficient of variation (CV) of the mechanical properties is suggested based on the parametric study.

1. Introduction

Progress in fabrication techniques has facilitated the manufacture of various nanoscale structures over the past decade. The potential functionality of nanostructures has caused great concern in various applications such as nanoscale electronic components, biochemical sensors, antibiotics, and higher functional catalysis [1–4]. Recently, it is possible to manufacture nano-thickness thin film made of the grain-free single-crystal copper by thermal atomic layer deposition [5]. Single-crystal copper is known for the high thermal and electrical conductivity. For electrical conductivity, the grain-free single-crystal copper shows better property than silver [6]. Meanwhile, porous structures such as heterogeneous foams or honeycombs have been designed for energy dissipation through large deformations [7]. Therefore, we focused on the nano-thickness thin film composed of the grain-free single-crystal copper including pores in this study.

The mechanical behavior in nanostructures is affected by the bonding loss at the free surfaces, which leads to size-dependent mechanical properties in nanostructures. This phenomenon is due to the asymmetric atomistic bonding at the free surface, and is called the surface effect. The surface effects can be captured by atomistic simulations, and molecular dynamics (MD) simulations among various atomistic simulations have been used conventionally to analyze nanostructures. However, since the simulation size in MD simulations is limited due to the high computation time and intensive resource requirements, MD simulations are intractable for practical design of submicron-scale structures.

Gurtin and Murdoch [8,9] first proposed the surface elasticity model, and their continuum approach combined with surface elasticity is very useful to analyze nanostructures. The continuum-based approach provides an alternative to overcome the limitations of MD simulations. For thin films with nano-thickness, Lim and He [10] and Lu et al. [11] derived a continuum model based on classical plate theory. The surface elasticity model serves as a bridge between the nanoscale and macroscale. Cho et al. [12] suggested a size-dependent continuum model with surface parameters extracted from MD simulations. Choi

* Corresponding author.
E-mail address: mhcho@snu.ac.kr (M. Cho).

http://dx.doi.org/10.1016/j.probengmech.2017.08.001
Received 7 March 2016; Accepted 1 August 2017
Available online 15 August 2017
0266-8920/

et al. [13] produced a thermo-elastic FE model considering the surface effects.

Homogenization methods have been applied to estimate the equivalent mechanical properties of heterogeneous structures. Generally, the homogenization methods have been assumed to have idealized periodicity of the composite or porous structures. Therefore, homogenized stiffness is predicted by a representative volume element (RVE). The two-scale homogenization is a kind of numerical method [14,15], and the effective mechanical properties of nanoscale porous materials [16] and micro/nano-sized honeycomb structures [17] can be predicted efficiently and reliably via two-scale homogenization by using the bridging technique. Cho et al. [18] studied the prediction of the mechanical properties of nanoparticulate composites by means of a homogenization method with the effective interphase concept. To solve large-scale complex-continuum heterogeneous micromechanics problems, Raghavan and Ghosh [19] proposed a multi-level model based on the homogenization method.

In real nano-scale structures, however, microscopic uncertainties such as those related to geometry and material properties are inevitable in the manufacturing process of periodic patterned structures. For this reason, the stochastic analysis for nano-thickness materials including patterned circular holes considering the microscopic uncertainties needs to be considered. Kaminski et al. [20] proposed a perturbation-based homogenization method for two-phase elastic composites for when there are uncertainties in the material properties of the fibers and matrix. Sakata et al. [21] considered geometric uncertainties by using an equivalent inclusion method based on micromechanics. Series expansion-based perturbation method is widely used in the stochastic finite element methods [22] and homogenization analysis [23]. Series expansion-based perturbation method is very efficient method because repetitive simulations such as Monte-Carlo simulation are not essential to obtain the stochastic responses. However, determining the coefficients of coupling terms between geometric variations is difficult. To avoid this drawback, structural perturbation method-based stochastic homogenization schematic is proposed in this study.

In this study, the stochastic characteristics of the mechanical properties of nano-thickness thin film structures including circular holes with geometric uncertainties in the size and distribution of holes are considered. The circular holes are arranged quasi-periodically. A multiscale framework with geometric uncertainty is proposed to identify the probability distribution of the homogenized elastic properties. A two-scale numerical homogenization method based on finite element analysis is used to obtain homogenized elastic properties. A Monte-Carlo simulation is performed to investigate the probability distributions of the elastic properties. Geometric uncertainties in the finite element models are handled by the moving-mesh generation technique [24]. A moving-mesh generation technique negates the need for repetitive remeshing procedures. Although Monte-Carlo simulation shows high accuracy for the multivariate stochastic system, it provides very low computational efficiency due to hundreds number of repetitive simulations. To overcome this drawback, reduced schematic is proposed by merging static reduction method and structural perturbation method with the Monte-Carlo simulation. The proposed reduced schematics show high efficiency. The previously developed bridging technique connecting a molecular dynamics unit cell model to a thin-film continuum membrane model was used to obtain the size-dependent mechanical properties exhibited at the nanoscale. In order to investigate the surface effects on the statistical characteristics for the nanofilm, the averages, standard deviations, and coefficients of variation (CV) of the mechanical properties obtained by the two-scale numerical homogenization are compared with those obtained without considering the surface effects. In addition, the influence of random volume fractions and the random distribution of holes on the mechanical properties were investigated. The parameters determining the CV of the mechanical properties are examined in the numerical examples. Lastly, guidelines to minimize the CV of mechanical properties are suggested based on the examined parameters.

2. Review of the continuum-based bridging model

This section provides the review of the continuum-based bridging model of nano-thickness thin film that merges the full atomistic MD simulation and finite element homogenization analysis [16], which is proposed by our group. To conduct stochastic homogenization analysis, this continuum-based bridging model is employed in this study.

2.1. The FE model considering the surface effects

Atoms on the free surfaces of a structure experience atomistic bonding loss. The atomistic bonding imbalance between the surface and the bulk parts causes size-dependency in the mechanical properties of nanostructures. For thin films, the upper and lower surface layers are introduced to express the asymmetric atomic bonding, as shown in Fig. 1. Each surface layer is assumed to adhere to the bulk layer perfectly. Thus, the continuity of displacement is satisfied at the interface between the surface and bulk layers as follows:

$$u_\alpha^{S^+} = u_\alpha\big|_{z=\frac{h}{2}}, \qquad u_\alpha^{S^-} = u_\alpha\big|_{z=-\frac{h}{2}}, \tag{1}$$

where S^+ and S^- denote the upper and lower surface layers, respectively.

The constitutive equation corresponding to the surface layers was firstly proposed by Gurtin and Murdoch [8,9]:

$$\tau_{\alpha\beta}^{S^\pm} = \tau_0\delta_{\alpha\beta} + (\mu_s - \tau_0)\left(u_{\alpha,\beta}^{S^\pm} + u_{\beta,\alpha}^{S^\pm}\right) + (\lambda_s + \tau_0)\, u_{\gamma,\gamma}^{S^\pm}\delta_{\alpha\beta} + \tau_0 u_{\alpha,\beta}^{S^\pm}, \tag{2}$$

where τ_0 is the surface residual tension, and λ_s and μ_s are Lamé's constants.

The Eq. (2) was derived for isotropic material, so it is not applicable to anisotropic materials. Single-crystal copper is an orthotropic material because its properties depends on the direction in which they is measured. Moreover, C_{1111} is equal to C_{2222} due to its symmetric geometry. Therefore, a modified constitutive equation, valid for single crystal structures [16], is represented as:

$$\tau_{\alpha\beta}^{S^\pm} = \tau_0\delta_{\alpha\beta} + \left(\left(\mu_s\right)_{\alpha\beta} - \tau_0\right)\left(u_{\alpha,\beta}^{S^\pm} + u_{\beta,\alpha}^{S^\pm}\right) + (\lambda_s + \tau_0)\, u_{\gamma,\gamma}^{S^\pm}\delta_{\alpha\beta} + \tau_0 u_{\alpha,\beta}^{S^\pm}, \tag{3}$$

where

$$\left(\mu_s\right)_{\alpha\beta} = \left(\mu_0^e - \mu_0^s\right)\delta_{\alpha\beta} + \mu_0^s. \tag{4}$$

The equilibrium equation for the nano-thickness thin film considering the surface effects can be derived via virtual work, and the procedure was presented in detail by Jeong et al. [16]. The internal virtual work consists of surface and bulk layer parts, and the term associated with the variation δu_α^0 yields the following equilibrium equation:

$$N_{\alpha\beta}^* = N_{\alpha\beta} + \tau_{\alpha\beta}^{S^+} + \tau_{\alpha\beta}^{S^-}, \tag{5}$$

where $N_{\alpha\beta} = \int \sigma_{\alpha\beta} dz.$, and $N_{\alpha\beta}^*$ is a newly defined in-plane force resultant.

By discretizing the displacement, the finite element model for the nano-thickness thin film is constructed as follows:

$$\mathbf{K} = \int_V \mathbf{B}^T\mathbf{C}\mathbf{B}dV + \int_A \mathbf{B}_{surf}^T\mathbf{C}^{surf}\mathbf{B}_{surf}\,dA, \tag{6}$$

where

$$\mathbf{C}^{surf} = \begin{bmatrix} 2\mu_0^e + \lambda_s & \lambda_s + \tau_0 & 0 \\ \lambda_s + \tau_0 & 2\mu_0^e + \lambda_s & 0 \\ 0 & 0 & \mu_0^s - \frac{1}{2}\tau_0 \end{bmatrix}. \tag{7}$$