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Size-dependent static characteristics of multicrystalline nanoplates by considering surface effects

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ABSTRACT

Nanostructures have been receiving extensive attention during the last two decades, due to their peculiar mechanical and other physical properties as compared with other macrostructures and macrosystems. The mechanical properties of nanostructures are intensely size-dependent. Furthermore, in the absence of external forces, nanostructures have a great tendency to deform due to their surface effects. Moreover, since the atoms on the surface have different equilibrium configuration from that of in the bulk, the elastic stiffness of the surface can be different from that of the bulk. In this study an ultra-thin plate of nanoscale thickness with an arbitrary geometry and boundary conditions is analyzed. A rectangular plate with nanoscale thickness is presented. In order to generalize the study, a multicrystalline plate with varying crystal properties has been assumed. Furthermore, the mechanical properties of the plate are dependent on the orientation. In fact the multicrystalline nanoplate is an anisotropic plate. The shapes and orientations of each crystal have been chosen haphazardly. However, the entire shape of the plate is a rectangle of microdimension with nanothickness. Due to the fact that silicon is much more applicable than any other material in Nanoelectromechanical systems (NEMS), it is assumed that the plate is made of silicon. The plate is subjected to a static load and the deformation as well as the corresponding strain is demonstrated. Due to the fact that the governing equation of the plate and its solution is not too straightforward to be solved easily, the finite element method is implemented so as to obtain the corresponding results. The results which have been achieved by the method of finite element and by employing the ANSYS software are illustrated and compared. Accordance of the results is quite remarkable.

1. Introduction

Mechanical properties and behavior of solids and structures are strongly size-dependent whenever the ratio of the surface area to the volume of the bulk becomes prominent. As a matter of fact, in nanoscale structures such as nanobeams, nanotubes, nanoplates, nanowires etc., due to their high ratio of the surface to the volume, the size dependency behavior of solids and structures cannot be overlooked. Moreover, the conventional theory of elasticity cannot be implemented due to size-dependence of a nanomechanical device. Consequently, in addition to the bulk properties presented in the theory of elasticity, surface effects namely surface elasticity (E^S), surface residual stress (τ^S) and surface mass density (ρ^S), will be described to define the mechanical behavior of nanostructures and devices.

Numerous theoretical research have been done on the surface effects. For instance, developing the conventional theory of elasticity by introducing surface elasticity was first elaborated by Gurtin and Murdoch in 1974 [1].

The mechanical quantity of surface effects for widespread materials was investigated by Shenoy [2]. Numerous authors studied surface effects in nanoplates and thin films. For instance, Stoney studied the effects of surface and interface stresses on the mechanical responses of thin films [3]. Moreover, changing the thickness of thin films breeds the changing of the Elastic Modulus. This investigation was elaborated by Cammarata and Sieradzki [4]. The size-dependent self-buckling and bending behaviors of nanoplates by considering surface effects was investigated by Wang and Zhao [5]. In spite of most contribution which neglects the residual stress, in this study the effect of residual stress which is induced by surface tension is considered. Guo and Zhao presented a theoretical model to investigate the size-dependent bending properties of nanobeams by considering surface relaxation as well as surface tension [6]. In this study the effective flexural rigidity and effective elastic modulus of a bending beam are derived. Thus, forecasting the mechanical properties and responses of nanoplates

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and thin films plays a leading role in the study of nanoplates. In addition to foregoing studies, numerous investigations have been elaborated based on the finite element method to determine the exact responses of nanoplates and thin films. Javili and Steinmann contributed the framework of the finite element method for the two-dimensional deformations of solids [7]. Furthermore, they contributed the framework of the finite element method for the three-dimensional case [8]. The Finite element method was formulated by Wang and coworkers for two-dimensional nanoscale structures by considering surface effects [9]. In order to investigate the size-dependent mechanical behavior in nanosystems, a finite element code was elaborated [10]. A similar investigation for a two-dimensional nanoscale structure in an elastic matrix was studied by Tian and Rajapakse [11]. The effect of grain size on the macro-young's Modulus and on the macro-Poisson's ratio was presented by Zhang and Sun [12]. The deformation of an elastic matrix as well as spherical nanocavities was studied by Yang [13].

In order for the equilibrium equations to be satisfied, it is shown that the existence of additional energies at the surface always changes the geometry of the nanostructures [14]. Several research were presented on the mechanical properties of silicon, which is a prevalent material in designing nanostructures and nanosystems. For instance, Young's Modulus, Shear Modulus and Poisson's ratio of silicon was studied by Wortman and Evans [15]. Jing and Meng studied the mechanical properties of crystalline silicon as well as amorphous silicon [16]. In addition, several investigations were presented in order to obtain the mechanical properties of amorphous silicon [17–21].

It should be noted that theoretical studies of this kind are strongly limited to systems of rudimentary geometry. Hence for systems of sophisticated geometry, it is far more suitable to use alternative methods such as the finite element method (FEM) instead of implementing conventional theoretical approach. With respect to this reason, the finite element method is implemented in this work. In this contribution we ponder over a multicrystalline nanoplate, which consists of several crystals with distinct orientation and static behavior of the multicrystalline nanoplate is investigated. In order to obtain the mechanical responses of the multicrystalline nanoplate, fundamental relations are derived and based on these relations, FEM codes are generated. The multicrystalline nanoplate behavior is simulated by employing the ANSYS software [22]. Finally, the results are compared and discussed.

2. Fundamental and governing equations

Fig. 1 shows a multicrystalline plate with width and length of microscale and thickness of nanoscale. Each crystal is assumed to be orthotropic and for this work this is an extraordinary presumption. It is important to note that these crystals are attached to each other by a region which is an amorphous of crystal materials. Amorphous phases are vital components of thin films and their material is analogous to the material of crystals. Due to the fact that the thickness of the plate is in the scale of nanometer, the ratio of the surface to the volume of the plate is high. Accordingly, surface effects cannot be neglected and consequently the fundamental equation of the surface must be taken into consideration in addition to the bulk equation.

2.1. Constitutive relations

From the theory of continuum mechanics, the orthotropic linear elastic behavior of the bulk can be mathematically described as

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{31}\\ \sigma_{12}\end{bmatrix}=\begin{bmatrix}\frac{1-\upsilon_{yz}\upsilon_{zy}}{E_yE_z\Delta} & \frac{\upsilon_{yx}+\upsilon_{zx}\upsilon_{yz}}{E_yE_z\Delta} & \frac{\upsilon_{zx}+\upsilon_{yx}\upsilon_{zy}}{E_yE_z\Delta} & 0 & 0 & 0\\ \frac{\upsilon_{xy}+\upsilon_{xz}\upsilon_{zy}}{E_zE_x\Delta} & \frac{1-\upsilon_{zx}\upsilon_{xz}}{E_zE_x\Delta} & \frac{\upsilon_{zy}+\upsilon_{zx}\upsilon_{xy}}{E_zE_x\Delta} & 0 & 0 & 0\\ \frac{\upsilon_{xz}+\upsilon_{xy}\upsilon_{yz}}{E_xE_y\Delta} & \frac{\upsilon_{yz}+\upsilon_{xz}\upsilon_{yx}}{E_xE_y\Delta} & \frac{1-\upsilon_{xy}\upsilon_{yx}}{E_xE_y\Delta} & 0 & 0 & 0\\ 0 & 0 & 0 & G_{yz} & 0 & 0\\ 0 & 0 & 0 & 0 & G_{zx} & 0\\ 0 & 0 & 0 & 0 & 0 & G_{xy}\end{bmatrix}\begin{bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ \gamma_{23}\\ \gamma_{31}\\ \gamma_{12}\end{bmatrix} \tag{1}$$

where

$$\Delta=\frac{1-\upsilon_{xy}\upsilon_{yx}-\upsilon_{yz}\upsilon_{zy}-\upsilon_{zx}\upsilon_{xz}-2\upsilon_{xy}\upsilon_{yz}\upsilon_{zx}}{E_xE_yE_z}$$

Because of having a plate of nanothickness, the case of plane stress exists. Thus, in the case of plane stress for an orthotropic material, Eq. (1) can be written

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{12}\end{bmatrix}=\begin{bmatrix}\frac{E_x}{1-\upsilon_x\upsilon_y} & \frac{\upsilon_xE_x}{1-\upsilon_x\upsilon_y} & 0\\ \frac{\upsilon_xE_x}{1-\upsilon_x\upsilon_y} & \frac{E_y}{1-\upsilon_x\upsilon_y} & 0\\ 0 & 0 & G_{xy}\end{bmatrix}\begin{bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \gamma_{12}\end{bmatrix} \tag{2}$$

where in this equation for simplicity υ_x and υ_y are expressed instead of υ_{xy} and υ_{yx}, respectively. Consequently for the bulk material, stiffness matrix can be expressed as

$$\sigma=[D]\varepsilon \tag{3 – 1}$$

$$[D]=\begin{bmatrix}\frac{E_x}{1-\upsilon_x\upsilon_y} & \frac{\upsilon_xE_x}{1-\ \upsilon_x\upsilon_y} & 0\\ \frac{\upsilon_xE_x}{1-\ \upsilon_x\upsilon_y} & \frac{\upsilon_xE_y}{1-\ \upsilon_x\upsilon_y} & 0\\ 0 & 0 & G_{xy}\end{bmatrix} \tag{3 – 2}$$

In order to derive a stiffness matrix for the surface of the plate like that for the bulk, Eq. (3-2), the linear surface stress–strain model, which was proposed by Gurtin and Murdoch [1] is considered

$$\sigma^s_{\alpha\beta}=\tau^0\delta_{\alpha\beta}+2(\mu^s-\tau^0)\varepsilon_{\alpha\beta}+(\lambda^s+\tau^0)\varepsilon_{kk}\delta_{\alpha\beta}\quad(\alpha,\beta=1,\ 2) \tag{4}$$

where $\sigma^S_{\alpha\beta}$ denotes the surface stress, λ^S and μ^S are Lame's constants of the surface, τ^0 is the residual surface stress at zero strain and $\varepsilon_{\alpha\beta}$

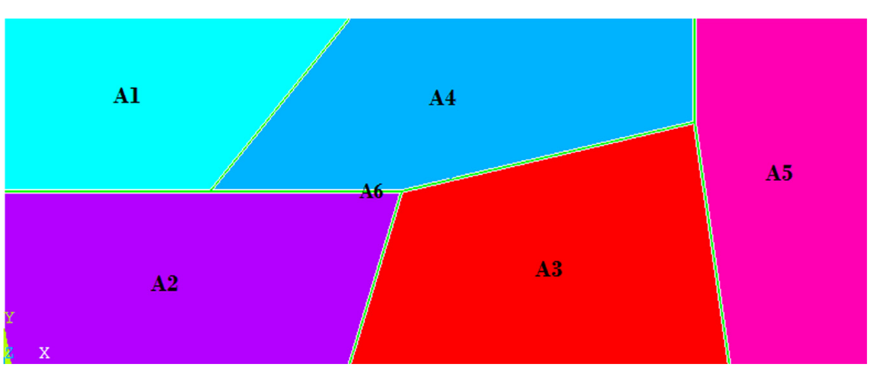

Fig. 1. Multicrystalline microplate with thickness of nanoscale and amorphous of nanowidth.