MODELING OF THIN COATED PLATES WITH MISMATCH DEFORMATION

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Summary Recent experimental studies have indicated the feasibility of a crystalline undulator obtained by depositing narrow periodic strips of silicon nitride on a silicon monocrystalline substrate. The residual stress associated to the deposition of silicon nitride induces a micro-undulation in the underlying silicon crystal. This communication reports on a research aimed at the mechanical modeling of the undulator structure and the characterization of the constitutive properties of the materials. In this direction, we first derive a total energy appropriate to describe the mechanical behavior of the three-dimensional film–substrate structure. Then, in order to find a two dimensional problem, we set up an approximating sequence depending on various scaling parameters. As a last step, we study the Γ–limit of the approximating sequence energy as the thicknesses of the substrate and the film tend to zero. By appropriately selecting the scaling parameters we deduce a two-dimensional (limit) energy suitable to describe the behavior of the film–substrate structure.

INTRODUCTION

Recently, it has been proposed a method to realize a crystalline undulator by depositing an alternate sequence of tensile strips of Si_3N_4 on a Si crystal, [1]. Indeed, since Si_3N_4 and Si have different thermal expansion coefficients and different lattice parameters, the manufacturing process induces a mismatch deformation between the Si_3N_4-film and the Si-substrate. This mismatch deformation, thanks to the eccentricity of the film and the alternate deposition of the Si_3N_4-strips, induces the undulation.
This communication reports on a research aimed at the mechanical modeling of a film–substrate structure, which bends because of a mismatch deformation, and at the characterization of the constitutive properties of the materials. In this direction, we first derive a total energy appropriate to describe the mechanical behavior of the three-dimensional film–substrate structure. Then, in order to find a two dimensional problem, we set up an approximating sequence depending on various scaling parameters. As a last step, we study the Γ–limit of the approximating sequence energy as the thicknesses of the substrate and the film tend to zero. By appropriately selecting the scaling parameters we deduce a two-dimensional (limit) energy suitable to describe the bending of the film–substrate structure due to the mismatch deformation between the film and the substrate.

MECHANICAL MODELING

Let $\omega \subset \mathbb{R}^2$ be a bounded open set with smooth boundary and let $\hat{h}^r$ and $\check{h}^r$ be two positive numbers. We denote by

$$\hat{\Omega}^r := \omega \times (0, \hat{h}^r), \quad \check{\Omega}^r := \omega \times (-\check{h}^r, 0),$$

the regions occupied by the film and the substrate in a chosen reference configuration, respectively. It could be shown that the energy, in a small deformation regime, of the film-substrate structure can be taken to be

$$\mathcal{F}^r(\mathsf{u}) = \int_{\hat{\Omega}^r} \mathring{\mathsf{T}}^r \cdot E\mathsf{u} + \frac{1}{2}\nabla\mathsf{u}\mathring{\mathsf{T}}^r \cdot \nabla\mathsf{u} + \frac{1}{2}\mathbb{L}^r(\mathsf{x})E\mathsf{u} \cdot E\mathsf{u}\, d\mathsf{x} + \int_{\check{\Omega}^r} \frac{1}{2}\mathbb{C}^r[E\mathsf{u}] \cdot E\mathsf{u}\, d\mathsf{x}, \tag{1}$$

where $\mathring{\mathsf{T}}^r$ is the stress induced by the mismatch deformation between the film and the substrate, $\mathbb{L}^r$ is the incremental elasticity tensor of the film and $\mathbb{C}^r$ is the elasticity tensor of the substrate. As usual, $\nabla\mathsf{u}$ denotes the gradient of u and $E\mathsf{u}$ is the symmetric part of $\nabla\mathsf{u}$. Since, in applications, $\hat{h}^r$ and $\check{h}^r$ are approximately equal to a few hundred nanometers and micrometers, respectively, while the diameter of ω is a few centimeters, it is quite natural to look for a two-dimensional energy which is in tight kinship with $\mathcal{F}^r$. More precisely, we are interested in finding a problem P_0 whose solution u_0 is close to the solution u^r of the real problem

$$\inf \mathcal{F}^r \qquad (P^r).$$

We shall achieve this by exploited modeling ideas developed in [2], which, briefly, consist in defining a sequence of problems P_ε such that:

1. P_ε variationally converges;
2. $P_{\varepsilon^r} = P^r$,

where $\varepsilon^r := \hat{h}^r/\mathrm{diam}\,\omega$. Indeed, by (1) we have that P_ε variationally converges to a problem P_0 whose solution is u_0. Since variational convergence implies that u_ε, the solution of the problems P_ε, converges to u_0, we have that u_ε is close

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to u_0 for ε small. But since ε^r is small, we have, by (2) that u^r, the solution of P^r, is equal to u_{ε^r} and hence u^r is close to u_0. Thus the solution of problem P_0 is close to the solution of problem P^r.
We now briefly sketch how we define the sequence P_ε by defining a sequence of energies $\mathcal{F}^\varepsilon$. For $\hat{h} = \check{h} = \text{diam}\,\omega$, let $\hat{\Omega} := \omega \times (0, \hat{h})$, and $\check{\Omega} := \omega \times (-\check{h}, 0)$. For $s > 0$ let

$$\hat{p}^\varepsilon(x_1, x_2, x_3) = (x_1, x_2, \varepsilon^{2s+1} x_3), \quad \text{and} \quad \check{p}^\varepsilon(x_1, x_2, x_3) = (x_1, x_2, \varepsilon x_3). \tag{2}$$

To every function $\mathsf{u} : \Omega^\varepsilon \to \mathbb{R}^3$ we associate two functions $\hat{u} : \hat{\Omega} \to \mathbb{R}^3$ and $\check{u} : \check{\Omega} \to \mathbb{R}^3$, defined by $\hat{u} := \mathsf{u} \circ \hat{p}^\varepsilon$, and $\check{u} := \mathsf{u} \circ \check{p}^\varepsilon$. With

$$\hat{H}^\varepsilon \hat{u} = \left(\partial_\alpha \hat{u} | \frac{\partial_3 \hat{u}}{\varepsilon^{2s+1}}\right), \quad \text{and} \quad \check{H}^\varepsilon \check{u} = \left(\partial_\alpha \check{u} | \frac{\partial_3 \check{u}}{\varepsilon}\right),$$

and $\hat{E}^\varepsilon \hat{u} := \text{sym}\, \hat{H}^\varepsilon \hat{u}$. and $\check{E}^\varepsilon \check{u} := \text{sym}\, \check{H}^\varepsilon \check{u}$. For $q, t, \eta \in \mathbb{R}$ and $s > 0$, let

$$\begin{aligned} \mathcal{F}^\varepsilon(\hat{u}, \check{u}) \;:=\; & \varepsilon^{2s} \int_{\hat{\Omega}} \varepsilon^t \overset{\circ}{T} \cdot \hat{E}^\varepsilon \hat{u} + \kappa \varepsilon^{t+q} \hat{H}^\varepsilon \hat{u} \overset{\circ}{T} \cdot \hat{H}^\varepsilon \hat{u} + \frac{1}{2\varepsilon^{2\eta}} \mathbb{L}[\hat{E}^\varepsilon \hat{u}] \cdot \hat{E}^\varepsilon \hat{u}\, dx \\ & + \int_{\check{\Omega}} \frac{1}{2} \mathbb{C}[\check{E}^\varepsilon \check{u}] \cdot \check{E}^\varepsilon \check{u}\, dx. \end{aligned} \tag{3}$$

It can be shown that κ, $\overset{\circ}{T}$, $\mathbb{L}$ and $\mathbb{C}$ may be chosen so that $\mathcal{F}^\varepsilon$ evaluated at $\varepsilon = \varepsilon^r$ is exactly equal to $\mathcal{F}^r/\varepsilon^r$, and hence $P_{\varepsilon^r} = P^r$. We may physically interpret the scaling parameters as follow: s takes into account the smallness of $\hat{h}^r$ with respect to $\check{h}^r$; t measures the intensity of the residual stress; η and q the rigidity of the film due to the material and the pre-traction, respectively, with respect to the rigidity of the substrate. By means of the theory of Γ–convergence we show that the right scaling parameters which describe the bending of the film–substrate structure due to a mismatch deformation are

$$t = -2s, \quad \eta = s \quad \text{and} \quad q \geq 2.$$

With these parameters the limit problem P_0 turns out to be defined by means of the energy:

$$\begin{aligned} \mathcal{F}(\xi, \xi_3) \;=\; & \int_\omega \hat{h} \overset{\circ}{T} \cdot \bar{E}\xi + \frac{1}{2}(\hat{h}\bar{\mathbb{L}} + \check{h}\bar{\mathbb{C}})\bar{E}\xi \cdot \bar{E}\xi\, dx + \\ & \int_\omega -\frac{\hat{h}\check{h}}{2} \bar{\mathbb{L}} \bar{E}\xi \cdot \bar{\nabla}^2 \xi_3\, dx + \\ & \int_\omega -\frac{\hat{h}\check{h}}{2} \overset{\circ}{T} \cdot \bar{\nabla}^2 \xi_3 + \chi_q \kappa \hat{h} \overset{\circ}{T} \bar{\nabla}\xi_3 \cdot \bar{\nabla}\xi_3 + (\frac{\hat{h}\check{h}^2}{8}\bar{\mathbb{L}} + \frac{\check{h}^3}{12}\bar{\mathbb{C}})\bar{\nabla}^2\xi_3 \cdot \bar{\nabla}^2 \xi_3\, dx, \end{aligned} \tag{4}$$

where $\chi_q = 1$ if $q = 2$, $\chi_q = 0$ if $q > 2$, $\bar{\nabla}$ and $\bar{E}$ denote the two dimensional gradient and strain, respectively, and

$$\bar{\mathbb{L}}(\cdot)[\bar{A}] \cdot \bar{A} := \inf_{b \in \mathbb{R}^3} \mathbb{L}(\cdot)[\bar{A} + b \odot e_3] \cdot (\bar{A} + b \odot e_3),$$

$$\bar{\mathbb{C}}(\cdot)[\bar{A}] \cdot \bar{A} := \inf_{b \in \mathbb{R}^3} \mathbb{C}(\cdot)[\bar{A} + b \odot e_3] \cdot (\bar{A} + b \odot e_3),$$

for every $\bar{A} \in \mathbb{R}^{2\times 2}_{\text{sym}}$. The field ξ describes the in-plane displacement of the plate, while ξ_3 denotes the out-of-plane displacement component. For large residual stresses the scaling parameter q should be set equal to 2.

References

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