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Atomic-Scale Modeling of Self-Positioning Nanostructures

Y. Nishidate[1], G. P. Nikishkov[1]

Summary

Nanoscale structures have many potential applications. However, controlling and manipulating formation of nanoscale structures is usually complicated. One promising approach to creation of 3D nanoscale structures exploits methods utilizing self-positioning phenomena of thin solid films. The self-positioning is caused by lattice mismatching strain in layered structures composed of several metal or semiconductor materials. The self-positioning structures are created by depositing a sacrificial material layer and several lattice-mismatched layers. After etching away the sacrificial layer, the layered materials form hinges or tubes with diameter controllable by layer material properties and thickness. Strain-driven self-positioning can be used to create 3D nanoscale structures by folding 2D membranes as *origami* (Japanese paper craft). This approach is simple and robust, and deformation is predictable and controllable.

Analytical continuum mechanics approaches and computational finite element modeling have been applied to estimating deformations of self-positioning multi-layer structures. However, these approaches do not take into account atomic-scale effects like absence of neighboring atoms at free surfaces.

Recently, the atomic-scale finite element method (AFEM) based on the Brenner interatomic potential has been proposed for multi-scale analysis of carbon nanotubes. We have applied the AFEM to modeling of self-positioning bi-layer structures. Investigation of curvature radius dependence on the structure thickness[2] showed that atomic-scale and continuum mechanics solutions produce same results for structures with thickness larger that 100 nm. Atomic scale effects play a significant role for thin self-positioning nanostructures.

In this paper, formulation of the atomic-scale finite element method with the use of the Tersoff-Nordlund potential function is presented. Since self-positioning of nanostructures involves large translations and rotations a special iteration procedure that includes a load relaxation factor is proposed. The developed AFEM code is applied to modeling of GaAs and InAs bi-layer self-positioning nanostructures. Two problem series include investigation of nanohinge curvature radius dependence upon structure thickness and material orientation angle. The self-positioning hinge deformation converges to the continuum mechanics solution under plane strain conditions with increasing structure thickness. However, for nanostructures

[1]University of Aizu, Aizu-Wakamatsu 965-8580, Japan

[2]Nishidate, Y. and Nikishkov, G. P. (2007): Effect of thickness on the self-positioning of nanostructures. *J. Appl. Phys.*, 102, pp. 083501–1–5.

of small thickness less than 40 nm, atomic-scale effects play considerable role. Dependency of curvature radius on material orientation angle shows periodic curve with the maximum curvature radius observed for orientation angle 45 degrees. Our modeling shows that hinges with different material orientation angles can exhibit curvature radii differing by up to 35%.