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Molecular dynamics simulation of spontaneous self rolling of (100)/(111) oriented bilayer aluminum nanofilms into nanotubes[1] DOREL MOLDOVAN, JIJUN LAO, Mechanical Engineering Department, Louisiana State University, Baton Rouge, Louisiana — We report molecular dynamics simulation studies that introduce a new methodology for forming metallic nanotubes and nanocoils via spontaneous self rolling-up of initially planar free standing (001)/(111) bilayer metallic nanofilms. Our studies on aluminum reveal that the self rolling of the bilayers is controlled by both energetic and kinetic processes accompanying the spontaneous structural reorientation of the top (001) layer to the (111) orientation of the substrate layer. The simulations indicate that the (001) to (111) reorientation of the top layer proceeds via nucleation from multiple sites and growth of the (111) oriented domains. While a newly formed (111) domain grows free of defects, a region containing a surface dislocation defect forms when two such domains meet. The bilayer reaches a lower energy state by undergoing multiple localized bendings of finite angles about the common direction that coincides with the corresponding surface dislocation line. The radii of the resulting structures are determined by bilayers thickness and temperature.

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