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Spontaneous Formation of A Nanotube From A Square Ag Nanowire: An Atomistic View[1] MINE KONUK ONAT, Department of Physics, Istanbul Technical University, Istanbul, Turkey, SONDAN DURUKANOGLU, Nanotechnology Research and Application Center, and Faculty of Engineering and Natural Sciences, Sabanci University, Istanbul, Turkey — We have performed molecular static calculations to investigate the recently observed phenomenon of the spontaneous formation of a nanotube from a regular, square Ag nanowire[1]. In the simulations, atoms are allowed to interact via the model potential obtained from the modified embedded atom method. Our simulations predict that this particular type of structural phase transformation is controlled by the nature of applied strain, length of the wire and initial cross-sectional shape. For such a perfect structural transformation, the <100> axially oriented fcc nanowire needs (1) to be formed by stacking A and B layers of an fcc crystal, both possessing the geometry of two interpenetrating one-lattice-parameter-wide squares, containing four atoms each, (2) to have an optimum length of eight layers, and (3) to be exposed to a combination of low and high stress along the length direction. The results further offer insights into atomistic nature of this specific structural transformation into a nanotube with the smallest possible cross-section. [1] M.J. Lagos et al., Nature Nanotech. **4**, 149 (2009).

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