Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

The structure and stability of thin H-passivated <112> silicon nanowires NING LU, Iowa State University, CRISTIAN CIOBANU, Colorado School of Mines, TZU-LIANG CHAN, University of Texas at Austin, CAI-ZHUANG WANG, Ames Laboratory, KAI-MING HO, Iowa State University, FENG-CHUAN CHUANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung, 804 TAIWAN — Recent experiments on the synthesis on monocrystalline nanowires reveal that their axis can only have a limited number of crystalline orientations. Among these orientations, <112> is the highest Miller-index wire axis and generates a rectangular cross-sectional shape. Using a combination between genetic algorithm search and density functional theory calculations, we determine the precise shape of the wire cross-section that corresponds to the lowest formation energy per silicon atom. We analyze the deviations of the cross-sectional shape from the Wulff shape, and show how the shape of the nanowires evolves as a function of cross-sectional area and the chemical potential of hydrogen.

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Date submitted: 03 Jan 2007 Electronic form version 1.4