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Mechanical and electronic properties at the interface between the Si(100) surface and semiconducting carbon nanotubes SALVADOR BARRAZA-LOPEZ, Virginia Tech — I discuss the *ab initio* mechanical and electronic properties of semiconducting carbon nanotubes adsorbed on the Si(100) surface. After revising results from nanotubes on the fully unpassivated surface[1], the interaction between a semiconducting nanotube and a fully H-passivated Si(100) surface with dopants is examined[2]. As silicon wafers are ordinarily doped, the model closely resembles experimental onditions[2,3,4], allowing for qualitative comparison. The single H-monolayer prevents electronic states in nanotubes from energetically shifting along with those of the doped supporting substrate, permitting the engineering of the relative positions of the slab and nanotube band edges. Finally, and following experimental work, we study adsorption characteristics of nanotubes on partially passivated surfaces. Surface states in the unpassivated regions modify the electronic structure of the interface and provide for the anchoring of nanotubes, deforming them in some cases. Results with and without dopants will be given[2].
1 S. Barraza-Lopez et al. J. Appl. Phys. (in press). 2 Submitted. 3 Appl. Phys. Lett 83, 5029 (2003). 4 P. M. Albrecht and J. W. Lyding, Small (in press).

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