Abstract Submitted for the MAR10 Meeting of The American Physical Society

Effective mass anomalies in strained silicon thin films JUN YA-MAUCHI, Keio University — The most fundamental shape of nanostructures may be a slab or thin film. Semiconductor slabs sandwiched insulators are a most basic model for the channel region of modern devices such as multi-gate and SOI (silicon on insulator) MOSFET. The aim of this presentation is to make systematic investigation of the shape effect on the electronic structures in the semiconductor slabs using a density functional pseudoptential method. Hydrogen terminated silicon thin films are used as a model of the slabs sandwiched by insulators. Adopted parameters are biaxial strain and crystal direction, as well as the thickness of the film. Among the calculated results, a remarkable feature is that the longitudinal effective mass component of the conduction band reveals anomaly on certain parameter lines in the < 110 > and < 111 > confinement cases. This anomaly is due to the confinement effect and lowering of the crystal symmetry by the strain. It is found that the confinement effect is semi-quantitatively explained by an extension of simple zero-point energy model using the first-principles k.p perturbation calculation. [1] J. Yamauchi, IEEE Electron Device Letters vol.29 186 (2008); J. Comp. Theor. Nanoscience (in press).

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Date submitted: 20 Nov 2009

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