Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles Study of the NiGe/Ge Schottky Barrier Height under Dopant Segregation[1] CHIUNG-YUAN LIN, Department of Electronics Engineering and Institute of Electronics, National Chiao Tung University, HAN-CHI LIN, R&D, Taiwan Semiconductor Manufacturing Company — Traditional Si-based MOSFETs are approaching its fundamental scaling limits, and Ge has been comprehensively explored as a potential channel material to replace Si due to its high intrinsic carrier mobility for further performance enhancement. Nevertheless, strong Fermi-level pinning near the valence band edge of Ge leads to high electron Schottky barrier height. Dopant segregation technique has been proposed to achieve shallower junction depth and heavier dopant concentration for NiGe/Ge. However, the role of dopants at the NiGe/Ge interface is not clear. In this study, first-principles calculations are employed to nail down the most stable dopant position and to obtain the physical Schottky barrier height (by HSE06 hybrid functional) of the NiGe/Ge contact. For the conventional n-type dopant such as phosphorous and arsenic, our calculations show that those two elements may be segregated at the interface, while the reduction of the Schottky barrier height is insignificant. This implies that the experimental improvement of the NiGe/n-type Ge junction by dopant are mainly attributed to the increased dopant concentration around the interface.

[1]The authors acknowledge financial support from the Taiwan Ministry of Science and Technology (under Grant No. MOST 103-2112-M-009-004-).

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Date submitted: 14 Nov 2014 Electronic form version 1.4