MAR08-2007-007456

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

Dangling-bond defects and hydrogen passivation in germanium

JUSTIN R. WEBER, Department of Physics, University of California, Santa Barbara, California 93106-9530, USA

The application of germanium in complementary metal-oxide semiconductor (CMOS) technology is hampered by high interface-state densities, the microscopic origin of which has remained elusive. Using first-principles calculations, we have investigated the atomic and electronic structure of prototype germanium dangling-bond defects [1]. The computational approach is based on density functional theory, and in order to overcome band-gap problems we have also performed quasi-particle calculations based on the GW approach. Surprisingly, the germanium dangling bonds give rise to electronic levels below the valence-band maximum. They therefore occur exclusively in the negative charge state, explaining why they have eluded observation with electron spin resonance. The associated fixed charge is likely responsible for threshold-voltage shifts and poor performance of n-channel transistors. At silicon/silicon dioxide interfaces, hydrogen is successfully used to passivate dangling-bond defects. We have therefore also investigated the interaction of hydrogen with germanium. In contrast to silicon and other semiconductors in which hydrogen behaves as an amphoteric impurity, interstitial hydrogen in germanium is stable only in the negative charge state, i.e., it behaves exclusively as an acceptor. Passivation of dangling bonds by hydrogen will therefore be ineffective, again explaining experimental observations. Other cases where unusual interfacial defects and problems with hydrogen passivation may occur will be discussed.

Work performed in collaboration with A. Janotti, P. Rinke, and C. G. Van de Walle, and supported by the Semiconductor Research Corporation.

1. J. R. Weber, A. Janotti, P. Rinke, and C. G. Van de Walle, Appl. Phys. Lett. 91, 142101 (2007).