

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Stability of donor-pair defects in $Si_{1-x}Ge_x$ alloy nanowires JI-SANG PARK, BYUNGKI RYU, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — Semiconductor nanowires (NWs) have attracted much attention because of the quantum confinement effect, large surface-to-volume ratio, and compatibility with the existing Si technology. Although impurity doping is important for applications to optoelectronic devices, it is generally difficult to dope nanostructures due to segregation of dopants to the surface, high activation energies induced by the surrounding low dielectric medium, and compensation by defects such as surface dangling bonds. Furthermore, compared with bulk Si, electrically deactivating donor-pair defects are energetically more favorable than isolated shallow donors in NWs. In this work, we perform first-principles density functional calculations to study the stability of donor-pair defects and the doping efficiency in $Si_{1-x}Ge_x$ alloy NWs doped with P impurities. The stability of donor-pair defects is enhanced as the Ge concentration increases. Consequently, the doping efficiency in $Si_{1-x}Ge_x$ alloy NWs is expected to be suppressed by the formation of donor-pair defects, similar to previous calculations for Si NWs with small diameters. The effects of reduced dimensionality, Ge chemical bonding, and strain on the stability of donor-pair defects in alloy NWs are discussed.

Ji-Sang Park
Dept of Physics, Korea Advanced Institute of Science and Technology

Date submitted: 13 Dec 2010

Electronic form version 1.4