

Abstract Submitted
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Confining P Diffusion in Si by an As-doped Barrier Layer LU-GANG BAI, GUANG-HONG LU, FENG LIU, Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT 84112, QI WANG, HAMZA YILMAZ, Fairchild Semiconductor, West Jordan, UT 84088 — We investigate the effect of As-doping on P diffusion in Si, using first-principles total-energy calculations. The formation of As-vacancy complex is found to be energetically favorable, which indicates the consumption of vacancy by As to prohibit vacancy-mediated P diffusion. In the vicinity of As-vacancy complex, the diffusion barrier of P via exchanging with Si vacancy is considerably increased, which further decreases the P mobility. These results qualitatively explain the experimental observations and provide useful direction for designing As-doped diffusion barriers for confining P diffusion in Si wafer processing and in MOSFET device fabrication.

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