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Schottky-Barrier height at Si(001)/PtSi(010) and Si(111)/$ErSi_2$(001) interface M.K NIRANJAN, S. ZOLLNER, L. KLEINMAN, A.A DEMKOV — According to the Si roadmap (ITRS) one of the most pressing concerns of CMOS technology beyond the 65 nm node is the contact resistances in source/drain regions between the doped silicon and silicide. For the 45 nm node it is expected to amount to one-fourth of the total parasitic resistance. This contribution will clearly only rise as the scaling continues. Thus the roadmap calls for a new contact technology by the 45 nm node. A monosilicide would have an additional advantage in lower Si consumption. The transition from $CoSi_2$ to NiSi is a step in that direction. Physically, the contact resistance comes from a relatively high Schottky-barrier between Si and silicide. For both $CoSi_2$ and NiSi the barrier is about 0.5 eV. Thus, it is desirable to identify new metals or alloys that will have lower Schottky barrier to n- and p- type Si for use in NMOS and PMOS, respectively. In deep submicron regime, PtSi, $ErSi_2$ and NiSi have been shown to be prospective candidates for replacing conventional silicides. We have studied the electronic structure of bulk PtSi and $ErSi_2$ within the framework of density functional theory. We then calculate work functions and surface energies for different surface orientations and come up with plausible interface structures with Si. Our calculated valance band Schottky-barrier height of 0.26 eV at Si(001)/PtSi(010) is in excellent agreement with the experiments. We have , also, calculated the valance band Schottky-barrier height of 0.29 eV at Si(111)/$ErSi_2$(001) interface.

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