Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Band Structure Engineering of PtSi[1] ALEX SLEPKO, ALEXANDER A. DEMKOV, The University of Texas — PtSi is being considered as a contact material in field effect transistors. It has an additional advantage of having a low Shottky barrier to p-type Si. The relatively low conductivity of PtSi compared for example to pure Pt can be traced to the low density of states at the Fermi level. In this theoretical study we discuss a method to increase the conductivity of PtSi by manipulating the density of states through alloying. The scheme is based on substituting Pt atoms by Ti atoms to shift the Fermi level to a higher density of states region. We find identify a compound with the carrier concentration 2.7 times larger than that of bulk PtSi. We estimate the formation energies of the compounds and determine the solubility limit of Ti in PtSi at room temperature. We analyze the effect of doping with Ti on the work function for the (121) surface (the lowest energy surface orientation of PtSi). Moreover, we study possible schemes to lower the formation energies of the alloys by further doping with boron, carbon, gallium and aluminum. We identify a stable alloy in the case of aluminum doping. All calculations are done within the framework of density functional theory.

[1]Supported by the Semiconductor Research Corporation under contract 2006-JV-1439

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Date submitted: 21 Nov 2008 Electronic form version 1.4