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First-principles study of the effects of Silicon doping on the Schottky barrier of $TiSi_2$/Si interfaces HAN WANG, Rensselaer Polytechnic Institute, EDUARDO SILVA, GLOBALFOUNDRIES, DAMIEN WEST, YIYANG SUN, Rensselaer Polytechnic Institute, OSCAR RESTREPO, GLOBALFOUNDRIES, SHENGBAI ZHANG, Rensselaer Polytechnic Institute, MURALI KOTA, GLOBALFOUNDRIES — As scaling of semiconductor devices is pursued in order to improve power efficiency, quantum effects due to the reduced dimensions on devices have become dominant factors in power, performance, and area scaling. In particular, source/drain contact resistance has become a limiting factor in the overall device power efficiency and performance. As a consequence, techniques such as heavy doping of source and drain have been explored to reduce the contact resistance, thereby shrinking the width of depletion region and lowering the Schottky barrier height. In this work, we study the relation between doping in Silicon and the Schottky barrier of a $TiSi_2$/Si interface with first-principles calculation. Virtual Crystal Approximation (VCA) is used to calculate the average potential of the interface with varying doping concentration, while the I-V curve for the corresponding interface is calculated with a generalized one-dimensional transfer matrix method. The relation between substitutional and interstitial Boron and Phosphorus dopant near the interface, and their effect on tuning the Schottky barrier is studied. These studies provide insight to the type of doping and the effect of dopant segregation to optimize metal-semiconductor interface resistance.

Han Wang
Rensselaer Polytechnic Institute

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