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Tight-binding based alloy scattering calculations in $\mathbf{Si_{1-x}Ge_x}$ SAUMITRA MEHROTRA, ABHIJEET PAUL, GERHARD KLIMECK — Role of alloy scattering in SiGe device performance has been up for debate since long time. The main source of confusion stems from the choice of alloy scattering potential parameter ΔU_{fit}. We present a theoretical model within tight-binding representation for treating alloy scattering in SiGe devices. The approach is shown to inherently capture the alloy scattering potential parameter(s) which otherwise are experimentally fitted or determined from first principles calculations for different band edges. It is shown that both onsite (variation in atom type) and off-diagonal (variation in bond type) blocks are important in estimating the potential value. The extracted scattering potential is then used to estimate bulk alloy scattering limited mobility in atomistic SiGe representation. The results show good agreement for both n-type and p-type experimental bulk mobility values.

Saumitra Mehrotra
Purdue University

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