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Study of Electronic Charge Distribution in Silicon Nanowire Transistors : An Atomistic Approach[1] ABHIJEET PAUL, SAUMITRA MEHROTRA, GERHARD KLIMECK, Purdue University — Atomistic modeling has been performed to investigate the spatial electronic charge distribution in silicon nanowire cross-sections. The modeling approach involves solution of electronic bandstructure using the 20 band sp3d5s* -SO nearest neighbor Tight-binding (TB) method with spin orbit (SO) interaction (LCAO) solved self-consistently with a two dimensional Poisson equation. Nanowires with rectangular, circular and triangular cross-section shapes have been investigated, with cross-section size of 3.1 nm and 5.1 nm for three different crystal orientations namely [100], [110] and [111]. The observed charge distribution as observed in these wires, is a strong function of cross-section shape, size and crystal orientation. [100] and [110] wires show strong corner effects, however, [111] oriented wires have centralized charge distribution. Charge distribution is sensitive to the structural and crystal symmetry of the nanowire. Structural confinement breaks the symmetry that manifests in the 1D energy dispersion of these wires by lifting up the degeneracy at the gamma valley. Finally, we enable the understanding of atomistic treatment for charge distribution in the capacitance measurements in these ultra-scaled silicon nanowire transistors.

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