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Atomistic Treatment of Electronic Transport: The Effect of Bandstructure[1] NEOPHYTOS NEOPHYTOU, ABHIJEET PAUL, GERHARD KLIMECK, Purdue University — The effect of bandstructrue on the electronic transport properties of nanowire devices is investigated using the sp3d5s*-SO 20-orbital nearest neighbor tight-binding model with spin-orbit interactions (LCAO), self consistently coupled to a Poisson solver for treatment of the electrostatics. Under strong spatial and electrostatic confinement at the nanoscale, atomistic effects become important. Non-parabolicity, anisotropy, band coupling, and valley splitting are evident in the electronic structure of these devices and strongly influence their transport properties. In addition to that, potential variations at the nanoscale also have strong influence on the device performance. It is shown that both the transport and quantization effective masses are a sensitive function of the device geometry and behave differently in different wire orientations. Under such conditions, traditional effective mass methods are inadequate and in general fail to describe device characteristics.

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