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Modeling transport through Si nanowires using a nonequilibrium Green function approach FABIANO OYAFUSO, PAUL VON ALLMEN, SEUNGWON LEE, GERHARD KLIMECK — We present our recent work in modeling electronic transport through Si nanowires using an nonequilibrium Green function approach. Our calculation, which extends the 1D nanoelectronic modeling software (NEMO) to 3D, uses a 20-orbital, orthogonal, semi-empirical tight-binding basis in which coupling between orbitals of nearest neighbor atoms are position dependent, so that lattice deformations and alloys can be accurately modelled. In this work, we study two effects on coherent transport through Si nanowires that are naturally included within this atomistic description. First, the sensitivity of the transmission coefficient due to surface perturbations is examined. A comparison is made between conductance through a hydrogen-passivated nanowire and one in which dangling bonds are introduced. Second, a study of transport through Si(x)Ge(1-x) barriers is presented. It is found that the transport behavior is markedly different from that in which a uniform material is assumed.

Fabiano Oyafuso
Jet Propulsion Laboratory

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