

Abstract Submitted  
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**Scattering Mechanisms in 3D Quantum Mechanical Simulations of a Silicon Quantum Wire**<sup>1</sup> MATTHEW GILBERT, RICHARD AKIS, DAVID FERRY, Arizona State University — We examine the inclusion of scattering processes in MOS quantum wires at room temperature, where phonon effects are prevalent. In a manner similar to Green's function approaches, but more amenable to the site representation used in these methods, scattering is computed on a mode basis and then transformed to the site basis. Beginning with the corresponding matrix elements, we derive mode to mode scattering rates for the different phonon processes and then perform a basis transformation to switch from mode space to real space. The resultant transformation gives us a complex matrix with terms that represent both the elastic and inelastic contributions resulting from the inclusion of different phonon processes. This matrix is then added into the pre-existing tight-binding Hamiltonian and the relevant transport quantities are calculated. Here, we present results of the first implementation of separable phonon scattering rates in a three-dimensional, fully quantum mechanical, self-consistent device simulation. The processes included are acoustic deformation potential scattering, intervalley absorption and emission containing both  $f$  and  $g$  type processes.

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