Microscopic Current Flow Patterns in Nanoscale Quantum Point Contacts

NA SAI, NEIL BUSHONG, University of California, San Diego, RYAN HATCHER, Vanderbilt University, MASSIMILIANO DI VENTRA, University of California, San Diego — Transport in nanoscale conductors has been studied extensively mainly using the stationary scattering approach. However, the dynamical nature of transport, and in particular, the flow patterns of the microscopic current through a nanoscale junction, have remained poorly understood. We apply a novel time-dependent transport approach [1], which combines closed and finite geometries with time-dependent density functional theory, to study current flow patterns in nanoscale quantum point contacts [2]. The results of both atomistic and jellium calculations show that surface charges form dynamically at the junction-electrode interfaces in both abrupt and adiabatic junctions. The current exhibits some characteristics of a classical hydrodynamic liquid but also displays unique patterns arising from the interaction with the surface charges. We also investigate the effect of the flow velocity, charge density, and lattice structures on the electron dynamics. If time permits we also discuss the effects of the viscosity of the electron liquid [3]. Work supported by DOE (DE-FG02-05ER46204). [1] M. Di Ventra and T.N. Todorov, J. Phys. Cond. Matt. 16, 8025 (2004). [2] N. Bushong, N. Sai and, M. Di Ventra, Nano Lett. (in press). [3] N. Sai, M. Zwolak, G. Vignale, and M. Di Ventra, Phys. Rev. Lett. 94, 186810 (2005 ).