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Modeling Sodium Nanowire's With Monte Carlo Simulated Annealing PEREYRA CARLOS, Cal State Univ - Sacramento, NANOWIRES TEAM — Building upon a Monte Carlo Simulated Annealing (**MCSA**) program, simulations were conducted on sodium nanowire's to determine and analyze how atoms arrange themselves in equilibrium. Previous calculations based on the quantum motion of conduction electrons have shown that only wires with "magic" radii are stable [3]. "Magic" conductance values 1, 3, 6, 12, 17, were modeled and the radial and pair distance distributions of these structures were analyzed. Radial distribution results show that structures form discrete shells, or radial regions, where atoms tend to reside, while pair distance distributions give information about the periodic arrangements of the atoms.Finding the optimal set of parameters in the program that allowed for structures with minimal amount of disorder while keeping the computation time reasonable was the objective of this project. This has proved sometimes closer to an art form than a systematic search. This has worked well for the smaller wires, but larger wires still remain rather disordered regardless of these changes.

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