Recent conductance data of Ni nanocontacts and break junctions revealed before breaking very small conductance steps [1,2], most likely corresponding to monatomic contact. The last step is near 1 (in units of $g_0 = e^2/h$, the conductance quantum per spin) for Ni nanocontact in a small magnetic field, and 2 in zero field which is anomalously small in comparison with the large expected number of $s + d$ conducting channels, of the order of 7 [3] even for a monatomic contact. We proposed recently [3] one of possible explanations of this result exploring the case of the Ni monatomic nanocontact where two tips are magnetized in opposite directions. Simulating the Ni nanocontact just as a monatomic regular infinite wire we showed that the insertion of a single magnetization reversal (a sort of collinear ”Bloch wall”) inside the monatomic magnetic nanowire leads to a sharp drop from 7 to 2 channels, a value now much closer to the experiments.

In order to make quantitative conductance predictions taking into account the real geometry of the nanocontact one needs to adopt a more detailed model comprising two semi-infinite metals (either thick wires or semi-infinite crystals) connected by a neck, a short monatomic wire, or just a single atom. For this purpose we have started to implement the approach proposed in Ref. [4] for calculating the ballistic conductance of open quantum systems within the Landauer-Buttiker theory. We generalize the original scheme to deal with ultrasoft pseudopotentials which adequately describe the nuclei and core electrons of a transition metal such as Ni. The important ingredient of the method is the one-dimensional complex band structure (composed of propagating and evanescent modes) of the perfect leads which is required in the wave function matching between the scattering region and the metallic electrodes. We present the complex band structure of fcc Ni and of a ferromagnetic Ni monoatomic wire and show that the method gives very accurate results for both the bulk solid and for the idealized monatomic nanowire. As a first example of conductance calculations the method is applied to the single atom carbon wires connected to aluminum electrodes where we are able to compare our results to earlier DFT calculations, based on nonequilibrium Green’s functions combined with a localized basis set [5,6].

References