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Structure and stability of suspended monatomic metal chains
ANWAR HASMY, NIST, Gaithersburg MD & Inest Group, PMUSA, Richmond VA, LUIS RINCON, NIST, Gaithersburg MD & ULA, Venezuela, RAIZA HERNANDEZ, IVIC, Venezuela, MANUEL MARQUEZ, VLADIMIRO MUJICA, NIST, Gaithersburg MD & Inest group, PMUSA, Richmond VA, CARLOS GONZALEZ, NIST, Gaithersburg MD — Since the spectacular achievement of the ultimately thin wire (a suspended monatomic gold chain) little progress has been made on the origin and the ubiquity of this phenomenon. Here we report a systematic quantum study on breaking monovalent metal nanowires through tight-binding molecular dynamics simulations. We show that at low temperature (4 K) gold, silver and copper can form linear and stable suspended monatomic chains at the late stage of the nanowire breaking process, but at room temperature silver and copper chains adopt a zigzag structure (as predicted by first principles calculations) that becomes unstable. We found that the stability and the average number of atoms forming these chains depend on the metal specie, a fact that can be explained in terms of the population of d-orbitals along the chains. Besides to clarify the controversy in the literature on the formation of these chains in 3d and 4d metals, our findings give insights on the advantages and limitations of detecting them through conductance measurements.

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