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On the Formation of Monatomic Metal Wires A. HASMY[1], NIST Center for Theoretical and Computational Nanosciences, Gaithersburg,MD, R. HERNANDEZ, Escuela de Quimica, UCV, Caracas, Venezuela, L.C. RINCON, Dpto. de Quimica, ULA, Merida, Venezuela, V. MUJICA, Escuela de Quimica, UCV, Caracas, Venezuela, R.J. MAGYAR, C. GONZALEZ, NIST Center for Theoretical and Computational Nanosciences, Gaithersburg,MD — The formation of monatomic metal wires under stress has been observed with HRTEM. It has been revealed that gold chains can be obtained if the stress is applied on the (111) and (100) orientations, while not on the (110) orientation. Other experiments have evidenced that some metals are unable to exhibit this monatomic wire formation. Theoretical efforts addressed to determine what are the geometrical and chemical conditions for such monatomic chain formations is still lacking in the literature. We have implemented Tight-Binding Molecular Dynamics simulations for the formation of metallic wires under stress, making special attention to the dynamics at the end of the contact breakage. Different geometrical orientations and chemical elements were considered. In order to determine the evolution of the electronic structure the simulations were complemented with *ab initio* calculations of the atomic configurations. The study allows us to give some insights about the required conditions for the formation of such monatomic metal wires.

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