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Theory and application for chain formation in break junctions YURIY MOKROUSOV, ALEXANDER THIESS, Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany, STEFAN BLUEGEL, Institut fuer Festkoerperforschung, Forschungszentrum Juelich, 52425 Juelich, Germany, STEFAN HEINZE, Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany — We introduce a generic model for chain formation in break junctions by formulating separate criteria for the stability and producibility of suspended monoatomic chains based on total energy arguments. Using first-principles calculations [1], we apply our model to break junctions of 4d and 5d transition-metals (TMs), as well as Ag and Au, including the effects of spin-polarization and spin-orbit coupling. Thereby, we can explain the physical origin of the experimentally observed trend of increasing probability for the creation of long suspended chains in break junctions for 5d-TMs at the end of the series [2] and suppressed chain elongation for 4d elements. Moreover, we clearify why the probability of chain elongation is greatly enhanced by the presence of oxygen in experiments with Au and Ag. Our model also allows us to make predictions on the ballistic transport properties of suspended chains. [1] Y.Mokrousov et al., Phys. Rev. B 72, 045402 (2005). [2] R.H.M.Smit et al., Phys. Rev.Lett.87, 266102 (2001).

> Yuriy Mokrousov Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

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