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Molecular dynamics study of the thermopower of Ag, Au, and Pt nanocontacts F. PAULY, Molecular Foundry, Lawrence Berkeley National Laboratory, USA, J.K. VILJAS, Department of Physics, University of Oulu, Finland, M. BÜRKLE, Institute for Theoretical Solid State Physics, Karlsruhe Institute of Technology, Germany, M. DREHER, P. NIELABA, Department of Physics, University of Konstanz, Germany, J.C. CUEVAS, Departamento de Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, Spain — Using molecular dynamics simulations of many junction stretching processes combined with tight-binding-based electronic structure and transport calculations, we analyze the thermopower of silver (Ag), gold (Au), and platinum (Pt) atomic contacts. In all cases we observe that the thermopower vanishes on average within the standard deviation and that its fluctuations increase for a decreasing minimum cross section of the junctions. However, we find a suppression of the fluctuations of the thermopower for the s-valent metals Ag and Au, when the conductance originates from a single, perfectly transmitting channel. Essential features of the experimental results for Au, Ag, and copper (Cu) of Ludoph and van Ruitenbeek [Phys. Rev. B 59, 12290 (1999)], as yet unaddressed by atomistic studies, can hence be explained by considering the atomic and electronic structure at the disordered narrowest constriction of the contacts. For the multivalent metal Pt our calculations predict the fluctuations of the thermopower to be larger by one order of magnitude as compared to Ag and Au, and suppressions of the fluctuations as a function of the conductance are absent. Main features of our results are explained in terms of an extended single-level model.

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