Abstract Submitted
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Ab-initio modelling of energy dissipation in nanotribological systems. A DFT study of fcc Cu(111) MICHAEL WOLLOCH, GREGOR FELDBAUER, Vienna University of Technology / Austrian Center of Competence for Tribology, PETER MOHN, JOSEF REDINGER, Vienna University of Technology, ANDRAS VERNES, Vienna University of Technology / Austrian Center of Competence for Tribology — Accurate modelling of the energy dissipation in sliding friction with *ab-initio* methods in nanotribological systems poses a fundamental challenge in modern tribology. Here we present a quasi-static model to obtain the nanofrictional response of dry, wearless systems based on quantum mechanical all electron calculations. We propose a mechanism for energy dissipation, which relies on the atomic relaxations during sliding. We define two different ways of calculating the mean nanofriction force, both leading to an exponential friction versus load behaviour for all sliding directions. Since our approach does not impose any limits on lengths and directions of the sliding paths, we investigate arbitrary sliding directions for an fcc Cu(111) interface and detect two periodic paths which form the upper and lower bound of nanofriction. For long aperiodic paths the friction force convergences to a value in between these limits. For low loads we retrieve the Derjaguin generalization of Amontons-Coulomb kinetic friction law which appears to be valid all the way down to the nanoscale. We observe a non-vanishing Derjaguin-offset even for atomically flat surfaces in dry contact.

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