Abstract Submitted
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Computer Simulation of Copper Nanowires[1] EDISON Z. DA SILVA, E.P. AMORIM, Instituto de Física "Gleb Wataghin", UNICAMP,CP 6165, 13083-970, Campinas - SP, Brazil, A.J.R. DA SILVA, A. FAZZIO, Instituto de Física, USP, CP 66381, 05315-970, São Paulo - SP, Brazil — Any device to operate, no matter how large or small, needs metallic contacts. The trend towards nano-miniaturization, with the development of nanodevices, will require the understanding of the behavior of metals at the nanoscale, especially gold and copper. Gold has received a lot of attention, while copper, also an important metal has not been studied as much. Recently the dynamical evolution of copper nanowires was observed with high resolution transmission electron microscopy (HRTEM) experiments [1]. We have performed tight binding molecular dynamics (TB-MD) simulations of copper nanowires under stress along some directions until their rupture. The TB-MD calculations have been show to be an excellent tool to study gold nanowires [2]. We present the time evolution of the structures, the formation of defects and the forces sustained by the nanowires. We discuss the possibility of the formation of short linear atomic chains before the breaking. Our results are in good agreement with experimental results. [1] J. C. Gonzalez, et al., Phys. Rev. Lett. **93**, 126103-1 (2004). [2] E. Z. da Silva, A. J. R. da Silva and A. Fazzio, Phys. Rev. Lett. **87**, 256102 (2001).

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