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Helical [110] gold nanowires make longer linear atomic chains EDGARD AMORIM, EDISON DA SILVA, Unicamp — Experiments performed on nanowires (NWs) synthesized by electron beam irradiation technique have shown that gold NWs formed along the [110] direction become helical when the NWs are sufficiently thin [1]. Moreover, helical and other non-crystalline structures have been theoretically predicted to other few metals [2]. Our study using tight-binding molecular dynamics show that gold NWs formed along the [110] direction reconstruct upon stress to form helical NWs. We discuss this formation and our results seem to indicate that an intrinsic mechanism is responsible for the formation of the helical structure. These helical NWs evolve on stretching to form linear atomic chains (LACs) and because they do not form symmetrical tips, these NWs produce longer LACs than other NWs. We use *ab initio* calculations to study the NW obtained from the tigth-binding simulations at stages close to rupture and compare LAC distances obtained with both methods. Furthermore, we investigate the electronic structure of the NW close to rupture [3]. [1] Y. Kondo, and K. Takayanagi, Science **289**, 606 (2000). [2] O. Gulseren, F. Ercolessi and E. Tosatti, Phys. Rev. Lett. **80**, 3775 (1998). [3] E.P.M. Amorim and E.Z. da Silva, Phys. Rev. Lett. **101**, 125502 (2008).

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