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Theoretical study of the morphology of stretched gold nanowires

FRANCESCA TAVAZZA, ANNE CHAKA, LYLE LEVINE, National Institute of Standard and Technology — Gold nanowires (NW) have been proposed for a variety of applications, including as intrinsic force standards in the nanoregime. To determine if they are effectively suitable for such an usage, we analyzed the dependence of the evolving NW morphology on different strain rates and directions, using semi-static, density functional (DFT) calculations. The NW under examination are very thin, initially fcc and have the wire axis along the (110) crystallographic orientation. The uniqueness of the necking pathway and the corresponding pre-failure structure are analyzed. The structure evolution and the ultimate length of the NWs are shown to be extremely sensitive to the tensile direction, and possibly on the strain rate as well, indicating that the corresponding energy surface is complex and that any experimental quantitative evaluation of the forces necessary to break the NW should keep parameters such as stretching direction and strain rate under careful control.

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