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Escape of an axial dislocation from a thin rod ZHAOXUAN WU, YONG-WEI ZHANG, MARK JHON, DAVID SROLOVITZ, Institute of High Performance Computing — Whiskers, nanowires and nanorods have been supposed to grow by preferential attachment to the atomic step formed from a screw dislocation intersecting the surface. This is expected to leave behind an axial screw dislocation, as has been observed in ionic nanowires such as NaCl, PbS and PbSe. However, we are not aware of any studies that have directly observed axial dislocations in pure FCC metal nanowires. To explain this, we speculate that thermal vibrations will be enough to kick out dislocations due to their high mobility. We consider two models of how a dislocation might escape from a nanowire. The first model is that the dislocation vibrates inside the nanowire. The second is that the nanowire itself vibrates, causing deformations of the nanowire that push the dislocation out. Analysis of these models imply that dislocations in thin nanowires are remarkably thermally stable. We test this prediction with molecular dynamics calculations on Cu nanowires, and find that the preparation of these systems is critical to the dislocation stability. Preparing the sample by simply raising the MD temperature will cause the dislocation to run out.

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