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单晶和多晶钼纳米丝轴向拉伸的模拟对比

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摘 要：利用分子动力学模拟研究多晶纳米丝和单晶钼纳米丝在拉伸形变行为上的差异。结果表明：单晶纳米丝比多晶纳米丝具有更高的弹性模量、屈服应力和断裂应变，且在拉伸过程中伴随更多的结构转变和无序化，导致超塑性的出现；多晶纳米丝拉伸时的颈缩从应力高度集中的晶界开始，结构转变也仅局限于此晶界附近，系统的整体结构几乎没有受到影响，且晶界处的高应力在控制多晶纳米丝的塑性形变和断裂过程中起着决定性的作用；纳米丝拉伸时由应力引起的结构转变也是塑性变形的一种重要机制。

关键字：钼纳米丝；结构转变；力学性能；分子动力学

Comparison of simulation of single-crystalline and polycrystalline Mo nanowires under uniaxial tensile strain

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Abstract: Using molecular dynamic simulations, the difference of tensile deformation behavior between the polycrystalline Mo nanowires and single-crystalline counterparts was investigated. The results show that, compared with the polycrystalline nanowires, the single-crystalline nanowires have higher elastic modulus, yield strength and fracture strain, and more local atomic structural evolutions and amorphization exist during tensile strain, which results in the superplasticity behaviors of single-crystalline nanowires. For the polycrystalline nanowires, the necking commences from the grain boundary regions of high stress concentration, and the local atomic structural transitions happen only near these regions. Thus, the degree of structure order is rarely affected with increasing strain. The high stresses found in the grain boundary regions of polycrystalline nanowires clearly play a dominant role in controlling both inelastic deformation and fracture processes in the nanoscale objects. The observed atomic configuration transformation is a stress-induced mechanism accounting for plastic deformation.
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