

Nb 在 Mo-Nb 合金辐照诱导硬化中关键作用的原子尺度研究

摘要

钼铌 (Mo-Nb) 合金因其优异的抗蠕变性和高真空功函数特性, 被认为是空间热离子反应堆能量转换部件的首选材料。然而, 溶质 Nb 原子引起的辐照硬化基本机制仍不明确。本研究通过分子动力学 (MD) 模拟, 探究了刃位错与 Nb 修饰辐照缺陷的相互作用, 并与辐照缺陷及富 Nb 团簇的作用进行了对比。模拟结果表明: Nb 在位错环上的偏析会显著影响这些环与刃位错的相互作用。当位错环被 Nb 修饰后, 特别是当环的取向平行于滑移面且相对于位错的伯氏矢量倾斜时 ($\langle 11\bar{1} \rangle$ 型环), 这些环会从弱障碍转变为强障碍。Nb 修饰的 $\langle 11\bar{1} \rangle$ 型环对滑移位错的钉扎强度还取决于 Nb 浓度。一旦 Nb 浓度超过临界值, 位错将无法吸收或剪切 $\langle 11\bar{1} \rangle$ 型环。此外, 临界 Nb 浓度随 $\langle 11\bar{1} \rangle$ 型环尺寸增大而升高, 这是因为 Nb 原子与位错环的平均结合强度随环尺寸增大而降低, 需要更高 Nb 浓度进行补偿。这些发现为理解 Mo-Nb 体系辐照硬化机制提供了新见解。

关键词

Mo-Nb 合金; 铌聚集; 辐照硬化; 刃位错滑移; 临界分切应力

Abstract

Molybdenum-niobium (Mo-Nb) alloys are considered the preferred materials for energy conversion components in space thermionic reactors because of their excellent creep resistance and high vacuum work function. However, the fundamental mechanism of irradiation hardening caused by solute Nb atoms remains unclear. Here, the interaction between edge dislocations and Nb-decorated irradiation-induced defects was studied using molecular dynamics (MD) simulations, and the results were compared to interactions with irradiation-induced defects and Nb-rich clusters. The simulation results showed that Nb segregation to loops greatly affects the interaction between these loops and edge dislocations. The loops can change from weak barriers to strong obstacles when decorated with Nb, especially when the loop orientation is parallel to the glide plane and inclined relative to the Burgers vector of the dislocation ($\langle 11\bar{1} \rangle$ loops). The pinning strength of Nb-decorated $\langle 11\bar{1} \rangle$ loops on gliding dislocations also depends on Nb concentration. Once the Nb concentration exceeds a certain critical level, the $\langle 11\bar{1} \rangle$ loops can no longer be absorbed or sheared by the dislocations. Additionally, the critical Nb concentration increases with $\langle 11\bar{1} \rangle$ loop size. This happens because the average binding strength between Nb atoms and loops decreases as $\langle 11\bar{1} \rangle$ loop size grows, requiring a higher Nb concentration to compensate. These findings offer new insights into the mechanisms behind irradiation hardening in the Mo-Nb system.

Keywords

Mo-Nb alloys; Nb aggregation; Irradiation hardening; Edge dislocation glide; Critical resolved shear stress

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