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分子动力学模拟金属玻璃压痕过程的应力晶化行为

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摘 要：采用Mishin镶嵌原子势，通过分子动力学方法模拟金属玻璃在压痕过程中的晶化行为，从微观结构演化的角度考察应力晶化过程中晶粒的形核、长大与合并的过程。局部较大剪切应力导致内部临近的非晶原子形成晶核，发生晶粒生长与合并的区域与Hertz理论符合。最终生成的晶粒具有面心立方结构，其(111)方向平行于剪切面。计算结果与文献中的实验现象一致，并且符合最小能量准则。

关键字： 金属玻璃；应力晶化；分子动力学；压痕

Molecular dynamics simulation of stress-induced crystallization behavior during indentation for metallic glass

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Abstract: The stress-induced crystallization behavior was simulated during the indentation deformation process for metallic glass copper using molecular dynamics method. The Mishin embedded atom method (EAM) was adopted as the interaction among atoms in the system. The nucleation, growth and coalescence of crystal grains were investigated through the evolution of microstructure. The local shear stress of amorphous system makes neighboring atoms nucleate. The site of growth and coalescence of crystal grains agrees well with the Hertz theory. The final crystalline phase has a FCC structure and the (111) plane is parallel to the shear direction. The computational result is consistent with the reported experiment phenomena and the minimum energy principle.

Key words: metallic glass; stress-induced crystallization; molecular dynamics; indentation

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