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单晶金属AFM切削过程的分子动力学模拟

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摘　要：

使用三维分子动力学方法模拟了基于AFM针尖的不同结构（FCC，BCC）的单晶金属（铝，铁，铜，镍）的纳米切削过程，研究了单晶金属延展性能对切削过程工件材料变形的影响。使用Morse势计算工件原子之间，工件原子和刀具原子之间的相互作用。观察和分析了切削过程中切屑形成，工件变形区域，以及系统势能变化。模拟结果显示单晶金属延展性能对基于AFM的纳米切削过程有显著影响。

关键词：纳米切削 AFM 分子动力学 单晶金属 延展性能

Molecular dynamics (MD) simulation of AFM-based nanometric cutting of some single-crystal cubic metals

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Abstract:

Molecular dynamics (MD) simulations of AFM-based nanometric cutting have been carried out on some single-crystal cubic metals, both FCC (Al, Cu, and Ni) and BCC (FCC) to investigate the effect of ductility of metal material on the nature of deformation during the nanometric cutting process. The Morse potential was utilized to compute both the interactions between workpiece atoms, interactions between workpiece atoms and tool atoms. Chip formation, workpiece deformation region, and system potential energy variation were observed. The results reveal that the AFM-based nanometric cutting process is significantly affected by the ductility of single-crystal metal material.

Keywords: nanometric cutting; AFM; molecular dynamics; single-crystal metal; ductility

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