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论文

单晶Cu材料纳米切削特性的分子动力学模拟

梁迎春,盆洪民,白清顺

哈尔滨工业大学机电工程学院, 哈尔滨 150001

摘要：

建立了单晶Cu纳米切削的三维分子动力学模型, 研究了不同切削厚度下纳米切削过程中工件缺陷结构和应力分布的规律. 纳米切 削过程中, 在刀具的前方和下方形成变形区并伴随缺陷的产生, 缺陷以堆垛层错和部分位错为主. 在纳米尺度下, 工件存在很大的表面应力, 随着切削的进行, 工件变形区主要受压应力作用, 已加工表面主要受拉应力作用. 随着位错在晶体中产生、繁殖及相互作用, 工件先后 经过弹性变形---塑性变形---加工硬化---完全屈服4个变形阶段, 随后进入新的循环变形. 结果表明: 工件应力--位移曲线呈周期性变化; 切削厚度较小时, 工件内部没有明显的层错产生, 随着切削厚度的增大, 工件表面和亚表层缺陷增加; 切削厚度越大, 对应应力分量值越小.

关键词： 单晶Cu 分子动力学 位错 应力分布 切削厚度

MOLECULAR DYNAMICS SIMULATION OF NANOMETRIC CUTTING CHARACTERISTICS OF SINGLE CRYSTAL Cu

LIANG Yingchun, PEN Hongmin, BAI Qingshun

School of Mechatronics Engineering, Harbin Institute of Technology, Harbin 150001

Abstract:

The increasing demand for designing and manufacturing micro parts with high quality comes from the high speed development of micro electromechanical systems (MEMS) and nano electromechanical systems (NEMS) in recent years. Nanometric cutting as an important machining way of micro parts has become a hot spot in machining field. Some main issues in nanometric cutting such as chip formation, machined surface quantity and diamond tool wear etc., have been investigated by molecular dynamics. Previous researchers have pointed out that the generation and evolution of defects are mainly responsible for causing plastic deformation of machined workpiece in nanometric cutting of plastic materials and a high compressive stress remaining in shear zone is considered beneficial to ductile–mode machining of brittle materials. Up to now, however, the influence of cutting thickness on defect behaviors and stress distribution in a workpiece and the relationship between them for single crystal materials are still unclear. In the present study, molecular dynamics simulations of nanometric cutting of single crystal Cu were performed. The simulation results show that stacking fault and partial dislocation are two main types of the defects in workpieces. A high surface stress at the atomc scale was observed in workpieces and there exist the compressive stress in shear zones and tensile stresses in the machined surfaces. It is found that the stress–distance curves of workpieces present a clear periodicity corresponding to the generation and evolution of dislocations in them. At he beginning of cutting (a small cutting thickness), no apparent stacking faults inside workpieces have been found, but with the increase of cutting thickness, the defects on surfaces and subsurfaces increase significantly and the thicker the cutting thickness, the smaller the corresponding stress components.

Keywords: single crystal Cu molecular dynamics dislocation stress distribution cutting thickness

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通讯作者: 盆洪民

作者简介: 梁迎春, 男, 1964年生, 教授, 博士

作者Email: hmpen23@126.com

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