

论文

单晶Cu纳米加工机理及其热效应的分子动力学模拟

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摘要:

基于大规模并行算法建立了单晶Cu纳米加工新型三维分子动力学仿真模型,采用Tersoff势、嵌入原子势(embedded atom method, EAM)和Morse势分别描述刀具原子之间、工件原子之间和工件与刀具原子之间的相互作用.研究了纳米加工过程中系统的温度分布及其热效应的影响,从位错和温度的角度对切屑形成过程和纳米加工表面的形成机理进行了分析.模拟结果表明:位错的扩展方向和切屑的堆积方向均沿着与切削方向成45°方向<110>晶向)运动;系统的温度分布呈同心形,切屑处温度最高,同时在金刚石刀具中存在较大的温度梯度;随着系统温度升高,工件材料具有热软化效应;切削速度和切削刃钝圆半径对系统的温度分布影响很大.

关键词: 单晶Cu 纳米加工 分子动力学 温度分布 热软化效应 位错

MOLECULAR DYNAMICS SIMULATIONS OF NANOMACHINING MECHANISM AND THERMAL EFFECTS OF SINGLE CRYSTAL Cu

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Abstract:

In recent years, nanomachining has received an increasing attention because of the remarkable advancement in sciences and technologies. In nanomachining process, the atomic interaction in surface and subsurface layers plays an important role. At such a small nanoscale, the traditional continuum representation method, such as finite element method, becomes questionable. This difficulty can be solved in general by molecular dynamics (MD). MD provides the necessary insight into nanomachining process and allows researching local material properties and behaviors in detail. Based on the large scale parallel algorithm, a new three-dimensional molecular dynamics simulation model was established for nanomachining of single crystal Cu. The interactions between workpiece atoms (Cu—Cu), copper and diamond atoms (Cu—C), and diamond atoms (C—C) were described by embedded atom method (EAM), Morse and Tersoff potentials, respectively. The temperature distribution and thermal effects during nanomachining were investigated. The chip formation and nanomachining mechanism were analyzed from the point of view of dislocation theory and thermal effects. The simulation results demonstrate that both the dislocation emission and chip pilep direction are along the h110i orientation. Temperature ditribution presents a roughly concentric shape and a steep temperature gradient lies in diamond tool, and the highest temperature is found in chip. The workpiece material becomes soft as the system temperature increases. Cutting speed and cutting edge radius have a significant effect on the system temperature distribution.

Keywords: single crystal Cu nanomachining molecular dynamics temperature distribution thermal soft effect dislocation

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