# Subsurface damage mechanism of high speed grinding process in single crystal silicon revealed by atomistic simulations

Jia Li[a,b], Qihong Fang[a,b*], Liangchi Zhang[c] , Youwen Liu[a,b]

[a] *State Key Laboratory of Advanced Design and Manufacturing for Vehicle Body, Hunan University, Changsha, Hunan Province, 410082, PR China*

[b] *College of Mechanical and Vehicle Engineering, Hunan University, Changsha, Hunan Province, 410082, PR China*

[c] *School of Mechanical and Manufacturing Engineering, The University of New South Wales, NSW 2052, Australia*

* *Corresponding author. Tel.:* +86 731 88822330*; fax:* +86 731 88822330*.*

E-mail address: fangqh1327@hnu.edu.cn; fangqh1327@tom.com

**Abstract**

Three-dimensional molecular dynamics (MD) simulations are performed to investigate the nanoscale grinding process of single crystal silicon using diamond tool. The effect of grinding speed on subsurface damage and grinding surface by analyzing the chip, dislocation movement, and phase transformation are studied. We also establish an analytical model to calculate several important stress fields including hydrostatic stress and von Mises stress for studying subsurface damage mechanism, and obtain the dislocation density on the grinding subsurface during nanoscale grinding. The results show that the higher grinding velocity results in larger chip volume and higher temperature in workpiece, and reduces subsurface damage. However, when grinding velocity above 180 m $s^{-1}$, subsurface damage thickness slightly increases because higher grinding speed increases grinding force and the temperature, which accelerate the dislocation nucleation and motion. Subsurface damage is studied by the evolution of surface area at first time for more obvious observation on transition from ductile to brittle, that provide valuable reference for machining nanometer devices. The von Mises stress and hydrostatic stress play an important role in the grinding processes, and explain the subsurface damage by the dislocation nucleation and motion in silicon under high stress. The plastic deformation induced dislocation nucleation and motion in silicon during grinding processes could better reveal subsurface damage mechanism considering stress and temperature acting on the dislocation.

**Keywords:** Nanoscale grinding; High speed grinding; MD simulation; Subsurface damage