The deformation mechanism of single crystal 6H-SiC under the nanoindentation and nanoscratching based on molecular dynamics simulations

Shuai Liu[1], Peipei Jing[1], Chaoqun Dang[1,#]

1 State Key Laboratory of Fluid Power and Mechatronic Systems, ZJU-Hangzhou Global Scientific and Technological Innovation Center, Center for X-mechanics, School of Mechanical Engineering, Zhejiang University, Hangzhou, China
Corresponding Author / Email:cqdang@zju.edu.cn

KEYWORDS: 6H-SiC, MD simulation, Dislocation, Phase transformation, Material removal

The silicon carbide (SiC) is a third-generation material with high thermal conductivity and breakdown electric field strength. However, the deformation behavior and damage mechanism of SiC during processing is still unclear. Hence, the international academic community has paid great attention to the mechanical properties of SiC. In recent years, nanoindentation and nanoscratching testing technologies have gradually become the mainstream testing method for the micromechanical properties of materials. However, the deformation behavior of the surface and subsurface for tested material is difficult to be monitored dynamically in real time in the process of nanoindentation and nanoscratching. In this paper, the nanomechanical properties of 6H-SiC are investigated by molecular dynamics (MD) simulation to unravel the mechanisms of elastic and plastic deformation under the nanoindentation and nanoscratching. Firstly, the MD model is established based on the previous experimental results, and then the surface morphology and crystal defects under the nanoindentation and nanoscratching are investigated, which are very difficult to realize in the experiments. The simulation results show that the amorphization of the 6H-SiC surface and the resulting dislocation slip are the two main modes of plastic deformation of covalent crystalline materials under nanoindentation and nanoscratching. During the loading process of the tool, the interatomic distances of the Si-Si atoms become shorter and preferentially bonded, resulting in the formation of a hexagonal atomic structure with fivefold coordination. Then the intermediate structure is rapidly transformed into an amorphous structure under further increase of tool displacement. The analysis of the dislocation types during the loading process shows that the atoms move along the <1-100> direction in the {0001} plane to form 1/3 <1-100> type dislocations. The MD simulation makes the mechanism of material plastic removal from the surface of 6H-SiC substrate clearer.