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Abstract:

Molecular Dynamics (MD) simulation has enhanced our understanding about ductile-regime machining of brittle materials such as silicon and germanium. In particular, MD simulation has helped understand the occurrence of brittle-ductile transition due to the high-pressure phase transformation (HPPT), which induces Herzfeld-Mott transition. In this paper, relevant MD simulation studies in conjunction with experimental studies are reviewed with a focus on (i) The importance of machining variables: undeformed chip thickness, feed rate, depth of cut, geometry of the cutting tool in influencing the state of the deviatoric stresses to cause HPPT in silicon, (ii) The influence of material properties: role of fracture toughness and hardness, crystal structure and anisotropy of the material, and (iii) Phenomenological understanding of the wear of diamond cutting tools, which are all non-trivial for cost-effective manufacturing of silicon. The ongoing developmental work on potential energy functions is reviewed to identify opportunities for overcoming the current limitations of MD simulations. Potential research areas relating to how MD simulation might help improve existing manufacturing technologies are identified which may be of particular interest to early stage researchers.

Keywords: MD simulation, silicon, diamond machining, high pressure phase transformation.