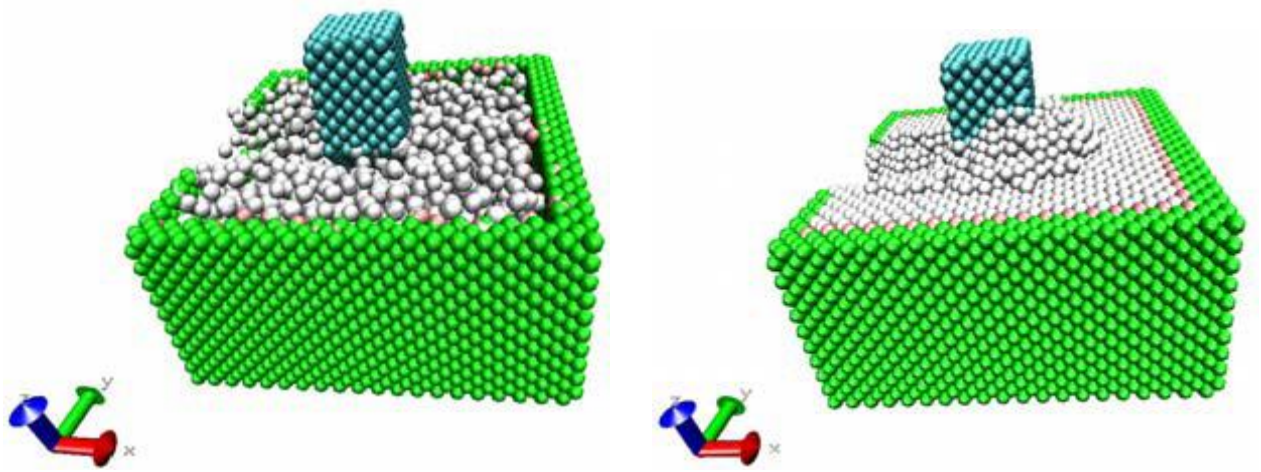
Imperfect Interatomic Potentials in the Molecular Dynamics Simulation of Copper and Diamond in Nanomachining

Akinjide Oluwajobi

Department of Mechanical Engineering, Obafemi Awolowo University, Ile-Ife, 220005, Nigeria email: j.oluwajobi@gmail.com and aogunjob@oauife.edu.ng



(a) (b)

Figure 1: Simulation results with (a) LJ potential (b) EAM potential

One crucial task in classical Molecular Dynamics (MD) simulation is the selection of appropriate interatomic potentials for the materials under investigation. If this is not properly done, it may lead to nonsensical results. In view of this, three popular interatomic potentials, namely the Lennard-Jones (LJ), Morse and Embedded Atomic Method, were used for the modeling of copper workpiece in nanometric machining. (The diamond cutting tool was treated as a rigid body). Figure 1 [1], [2] clearly shows the effects of the various potentials in the simulation. The EAM appears to model the copper atoms most accurately, as it best describes the metallic bonding of the atoms.

In other set of simulations, the effect of interatomic potentials on the prediction of the onset of plastic deformation in nanomachining was studied [3]. The pile-up volume and the force ratio were indicative of the onset of plasticity during the machining. The pile-up volume showed that ploughing starts from around 0.2 – 0.3nm, whereas the force ratio predicted the onset of plastic deformation from 0.1nm – 0.3nm. Also, the effects of interatomic potentials on the determination of the minimum depth of cut in nanomachining were investigated [4]. It was observed that the formation of chip initiates from the depth of cut thickness of 1.5nm. It is evident that for the MD method to be a viable predictive tool, suitable potentials are needed and the simulation results must be validated by experiments.

[1] A.O. Oluwajobi and X. Chen, Int J. Abrasive Technology 3 (2010) 354-381.
[2] A. Oluwajobi and X. Chen, Int. J. of Automation and Comp. 8 (2011) 326-332.
[3] A. Oluwajobi and X. Chen, Key Eng. Materials 535-536 (2013) 330-333.
[4] A.O. Oluwajobi and X. Chen, Int J. Abrasive Technology 6 (2013) 16-39.