Atomistic Modelling of Materials in Nanomachining

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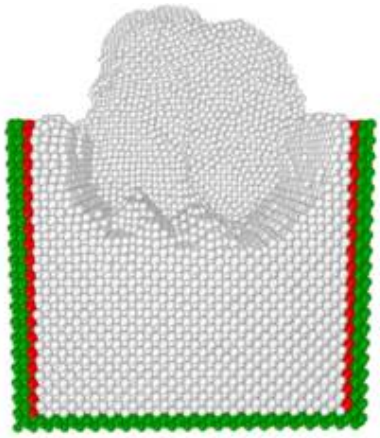

Figure 1: Nano Surface Created through MD Multipass Simulations

Many materials are employed in nanomachining; such as copper and aluminium, used as workpiece materials; and diamond and cubic boron nitride, used as the cutting tools materials. The interatomic potentials used in the atomistic modelling of these materials during nanomachining are reviewed and the associated material removal mechanisms are highlighted.
Futhermore, multi-pass nanometric atomistic simulations were carried out, with a diamond tool on a copper workpiece to create nano surfaces and the results provide the platforms from which the atomic surface roughness were evaluated. The estimated surface roughness (Sa) was in the order of 0.3 nm, but the value varies with the depth of cut and cutting velocity. It is essential that MD simulation results should be validated, and the evaluation of the surface roughness in this work, allows for comparisons with theory and experiments [1].

[1] A.O Oluwajobi, X.Chen, *Key Engineering Materials*, **2016**, *686*, 200-203.

Keywords: Interatomic Potentials, Molecular Dynamics, Nanomachining, Materials Removal Mechanisms