LUND UNIVERSITY

LTH
FACULTY OF ENGINEERING

Master of Science In Engineering, Engineering Physics

Modelling of nanometric cutting in metals using MD simulations

Popular Science Summary

by Damien Gautier

23rd September 2022

FMEM01
Degree Project in Mechanics for Engineers
September 2022

Popular Science Summary

Modelling and studying the nanometric cutting of a copper workpiece.

Because of the nanometric scale involved, this project cannot rely on classical theories of continuum mechanics but uses instead molecular dynamics to model the cutting of a piece of copper by a diamond tool.

In this master thesis project, a Molecular Dynamics simulator called LAMMPS was used to model the behaviour of atoms in a copper workpiece and in a diamond tool. This software models the copper-copper interactions in the workpiece, the carbon-carbon interactions in the tool and the copper-carbon interactions at the contact zone between these two parts. Because of the large number of atoms involved and the number of timesteps needed to model the whole cutting process, the code needed several days or weeks to run.

A previous study had already modeled the cutting of a copper piece for the same type of geometry but without having modeled the interactions of the carbon atoms within the diamond tool. The very first simulations have therefore served to highlight the importance of modeling these interactions to get a result closer to reality.

Then, the influence of several parameters was studied, like the cutting depth, the height of the workpiece or the tool radius. It turns out that the more dislocations there are in the workpiece, the more rigid it becomes and consequently the forces required to perform the cut and the temperature of the material increase. These results were observed on a software program called OVITO, acronym for Online Visualisation Tool, which allowed to visually see the evolution of material parameters during the cutting process, which was quite convenient.

Another calculation simulated three consecutive cuts of the same material, and this also highlighted the fact that the forces and temperatures involved increase cut after cut, which is an important element to take into account during machining processes.

Future work can continue the results of this master thesis and study more parameters, such as the orientation of atoms in the copper workpiece and the diamond tool, which was already studied briefly in this project but which deserves a more thorough study. The addition of grains in the structure of the studied materials could also be interesting in order to model them in a more realistic way.