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Effects of lubrication on friction and heat transfer in machining processes on the nanoscale: a molecular dynamics approach

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Abstract

Working fluids play an important role in machining processes. They serve twofold: On the one hand, they reduce the friction and thus weaken the generation of heat in the machining process. On the other hand, the working fluid cools the workpiece and the tool, acting as a heat sink. Both functionalities are investigated in the present work for a nanometric machining process by means of molecular dynamics simulations. The action of the tip of a cutting tool on a workpiece is studied both with and without working fluid. The Lennard-Jones truncated and shifted model is used for describing all interatomic interactions. The simulation results show that even in the presence of the working fluid, the tip of the cutting tool and the workpiece are mostly in direct contact during the machining process, i.e. the initially present fluid molecules are squeezed out of the contact zone. The work that is needed for the nanometric machining process is not significantly reduced by the fluid, but the coefficient of friction is. This results from a reduction of the normal force acting on the cutting tool. As expected, the working fluid has an important influence on the heat transfer during the nanometric machining process. Accordingly, mechanical quantities depend weakly on the solid-fluid interaction energy while the thermal quantities are more significantly influenced. The results of the study give insight in nanoscale phenomena in the contact zone between the tip of a cutting tool and the workpiece which cannot be studied experimentally.

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1. Introduction

The small zone in which the cutting tool and the workpiece are in direct contact in machining processes is hard to study experimentally, so that up to now there is only little information on the phenomena which occur in that highly important zone. Molecular dynamics simulations can provide such information. System sizes which are accessible by those simulations are presently typically on the nanoscale, even though with world record simulations the macroscale has yet been reached [1].

The nanoscale is also becoming directly relevant for the modern micro- and precision machining technology. E.g. in manufacturing of optical and photonic products tolerances in the order of nanometers must be met [2]. Processes on the nanoscale are governed by different effects compared to the corresponding processes at greater length scales. It is, e.g., well known from studies of fluid flow that on the nanoscale interfacial effects, which are negligible on larger scales become dominant [3].

In molecular dynamics simulations Newton's equations of motion are solved for an atomistic many-particle system. The interactions of the particles are described by classical force fields. For a given force field, only the scenario which is to be studied has to be specified. There are no assumptions or parameters, so that the simulation is completely predictive. Due to the strong physical background of the method, molecular dynamics simulations are often used in situations where the predictive power matters [4–7].

Molecular dynamics simulations have been used since the late 1980s [8] for studying tool-workpiece interactions. However, in most of these studies only the dry contact was studied, i.e. the tool and the workpiece interacted in a vacuum; see, e.g., [9–14]. The focus of these studies was on

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chip formation and the generation of dislocations in the workpiece.

It is, however, well known from macroscopic studies that machining processes are significantly influenced by cooling and lubrication by working fluids [15, 16]. There are up to now only a few molecular simulation studies which have addressed this [2, 17–21]. In these studies, typically a single solid-fluid pair is investigated, and no special attention is given to the influence of the solid-fluid interaction, even though that controls the contact angle and the wetting behavior in general [22, 23]. Furthermore, the thermal effects are usually not in the focus of the available studies. Therefore, in the present work, a molecular dynamics study of the effect of the working fluid on nanometric machining processes is carried out using a model system that enables systematic studies of the influence of the solid-fluid interaction. Both the mechanical and the thermal effects of the working fluid are studied by comparing the case with working fluid to the corresponding dry case.

2. Modeling and Simulation Setup

2.1. Molecular Model

The studied system consists of a workpiece, i.e. a solid substrate (S), the tip of a cutting tool (T), and eventually the working fluid (F). The tip is rigid, its movement is prescribed. All interactions are modeled with the Lennard-Jones truncated and shifted (LJTS) potential $u^{\mathrm{LJTS}}(r_{ij})$, i.e. those between the alike sites S-S and F-F, as well as the unlike interactions S-F, T-F, and S-T.

The LJTS model is well suited for describing properties of simple nonpolar fluids [3, 24], but it is only a crude model for solids. We use it throughout because we carry out a study of basic effects for which simplicity is beneficial. Furthermore, we can build on a recent study of the wetting behavior of LJTS walls by LJTS fluids [22]. The LJTS potential is [24]:

$$u^{\mathrm{LJTS}}(r_{ij}) = \begin{cases} u^{\mathrm{LJ}}(r_{ij}) - u^{\mathrm{LJ}}(r_{\mathrm{c}}), & r_{ij} < r_{\mathrm{c}} \\ 0, & r_{ij} \geq r_{\mathrm{c}} \end{cases}, \tag{1}$$

where

$$u^{\mathrm{LJ}}(r_{ij}) = 4\varepsilon[(\sigma / r_{ij})^{12} - (\sigma / r_{ij})^{6}], \tag{2}$$

Here, ε is the energy parameter, describing the dispersive attraction. σ is the size parameter describing the repulsion. r_{ij} is the distance between two LJTS sites i and j, and r_{c} is the cut-off radius, which is the maximal distance for which the attraction is considered.

The parameterization of the LJTS model for the different interactions, which was chosen here, results from preliminary runs with different parameterizations. The fluid model can be considered as representing a nonpolar liquid. The cohesion energy of the solid then corresponds to energies as they are observed in typical metals like iron or vanadium [25].

All sites have the same mass M. The size parameter σ is used to normalize all distances. Moreover, σ is the same for all LJTS sites. The cut-off radii of all alike and unlike interactions are $2.5\,\sigma$, except of the substrate-tool interaction that was kept purely repulsive by setting its cut-off to $r_{\mathrm{c,ST}} = 1.0\,\sigma$ [26]. All energies are normalized using the LJTS energy parameter of the fluid $\varepsilon = \varepsilon_{\mathrm{F}}$. The cohesive energy of the substrate is set to $\varepsilon_{\mathrm{S}} = 52\,\varepsilon_{\mathrm{F}}$. For the substrate-fluid and the tool-fluid interactions the cohesive energy is $\varepsilon_{\mathrm{SF}} = \varepsilon_{\mathrm{TF}} = 0.5\,\varepsilon_{\mathrm{F}}$. According to *Becker et al.* [22], this corresponds to a contact angle of about 90°. In follow-up work a systematic variation of the contact angle will be carried out.

All observables presented in that work are given in reduced units, cf. Table 1. Here, k_{B} is the Boltzmann's constant and the asterisk indicates the observables carrying a dimension.

Table 1. Characteristic system properties in quantities carrying dimensions.

Length	$x = x^* / \sigma$
Mass	$m = m^* / M$
Density	$\rho = \rho^* \sigma^3$
Time	$\tau = \tau^* / \left(\sigma\sqrt{M / \varepsilon}\right)$
Temperature	$T = T^* / (\varepsilon / k_{\mathrm{B}})$
Pressure	$p = p^* / (\varepsilon / \sigma^3)$
Velocity	$v = v^* / \left(\sqrt{\varepsilon / M}\right)$
Force	$F = F^* / (\varepsilon / \sigma)$
Work	$W = W^* / \varepsilon$
Thermal conductivity	$\lambda = \lambda^* / \left(k_{\mathrm{B}} / \left(\sigma^2\sqrt{M / \varepsilon}\right)\right)$

2.2. Simulation Scenario

A snapshot from a simulation is depicted in Fig. 1. For a better visualization, only a detail of the entire simulation box is shown. The simulation box contains the tip of a cutting tool modeled as a rigid cylinder with the radius $R = 9$ and the length $L = 71$, a solid substrate, and eventually a working fluid. The entire simulation box has the dimensions $l_{\mathrm{x}} = 309$, $l_{\mathrm{y}} = 71$ and $l_{\mathrm{z}} = 295$. For the case with working fluid it includes a total number of $4.89 \cdot 10^6$ LJTS. The number of sites assigned to the different objects is: substrate $3.16 \cdot 10^6$, the cutting tool $1.67 \cdot 10^4$, and the working fluid $1.71 \cdot 10^6$, if applicable.

The coordinate system used for the following discussion is indicated in Fig. 1. On the horizontal axis, $x = 0$ indicates the initial position of the midpoint of the cutting tool, which is constant during the indentation. On the vertical axis, $z = 0$ indicates the position of the midpoint of the cutting tool when its distance from the initially flat substrate surface is equal to R, i.e. when cutting tool and surface firstly touch in the dry case scenario. In the initial situation, the substrate is a crystal with a fcc lattice and the particle density $\rho_{\mathrm{S}} = 1.07$.

Periodic boundary conditions are applied in all directions, except for the fluid for which in z-direction a soft repulsive boundary condition is used. The two layers of substrate sites next to the box margins in x-direction and at the bottom of the box are fixed. A velocity scaling thermostat acts on the three layers of LJTS substrate sites next to the fixed layers, so that their temperature is kept at $T = 0.8$ throughout the entire simulation. That temperature is equivalent with the initial temperature of the system after the equilibration. The initial pressure is $p = 0.005$. During the whole process, no evaporation is observed in the fluid.