



Molecular Dynamics Simulation of Cutting Processes: The Influence of Cutting Fluids at the Atomistic Scale

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Abstract. Molecular dynamics simulations are an attractive tool for studying the fundamental mechanisms of lubricated machining processes on the atomistic scale as it is not possible to access the small contact zone experimentally. Molecular dynamics simulations provide direct access to atomistic process properties of the contact zone of machining processes. In this work, lubricated machining processes were investigated, consisting of a workpiece, a tool, and a cutting fluid. The tool was fully immersed in the cutting fluid. Both, a simple model system and real substance systems were investigated. Using the simplified and generic model system, the influence of different process parameters and molecular interaction parameters were systematically studied. The real substance systems were used to represent specific real-world scenarios. The simulation results reveal that the fluid influences mainly the starting phase of an atomistic level cutting process by reducing the coefficient of friction in this phase compared to a dry case. After this starting phase of the lateral movement, the actual contact zone is mostly dry. For high pressure contacts, a tribofilm is formed between the workpiece and the cutting fluid, i.e. a significant amount of fluid particles is imprinted into the workpiece crystal structure. The presence of a cutting fluid significantly reduces the heat impact on the workpiece. Moreover, the cutting velocity is found to practically not influence the coefficient of friction, but significantly influences the dissipation and, therefore, the temperature in the contact zone. Finally, the reproducibility of the simulation method was assessed by studying replica sets of simulations of the model system.

1 Introduction

Understanding the fundamental mechanisms of lubricated tribological processes on the atomistic scale is crucial for many technical applications such as cutting and grinding in manufacturing. Cutting fluids are used for two reasons: a) reduce the friction and b) reduce the heat impact and temperature of the workpiece. The fundamental mechanisms

in the small contact zone between a tool, a workpiece, and a lubricant behind these are today not fully understood. However, understanding these processes on the atomistic scale can be helpful for improving the macroscopic process, e.g. for modern micro- and precision machining technology. In-situ experimental investigations of the fundamental mechanisms on the atomistic scale are not possible today. As an alternative, classical molecular dynamics (MD) simulations can be used to gain insights into lubricated tribological processes on the atomistic scale. Due to the strong physical basis, molecular simulations can be applied in two general ways: a) the prediction of thermophysical properties of matter and b) modelling nanoscopic processes. In this work, the focus is on the modeling of nanoscopic cutting processes using molecular dynamics simulation.

Molecular simulations are based on solving Newtons equation of motion for an atomistic many particle system – considering boundary condition imposed by the simulation scenario, e.g. the movement of a tool. The interactions between the particles on the atomistic level are defined by force fields. Force fields aim at representing the molecular interactions and structure of a given real substance and, hence, mostly provide a reliable representation of the behavior matter. Besides using force fields for real substances, model systems can be favorably used in molecular simulation to study the link between molecular interaction parameters and macroscopic properties for obtaining generic information on processes [36, 35, 17, 4, 14, 33, 28]. Thereby, model systems can be used to study the fundamental mechanisms of complex processes in detail [8, 18, 13, 19, 9]. The Lennard-Jones model system is the most popular and widely used model system [34, 37]. In this work, both real substance systems and Lennard-Jones model systems were used for studying the atomistic processes of lubricated cutting.

In the literature, there are several MD studies available investigating the deformation of a workpiece and material removal caused by a tool, e.g. Refs. [36, 11, 1, 25, 27, 32, 39, 38]. However, in most studies, only dry contact processes (no cutting fluid) are considered, e.g. on the influence of the shape of the tool [2, 10] and the solid material [17, 11, 3, 42, 16]. The influence of cutting fluids is considered in only few studies, e.g. Refs. [39, 45, 26, 30, 31, 6].

In this work, the influence of cutting fluids on cutting processes were investigated on the atomistic scale. Thereby, different aspects of a cutting process were investigated such as the behavior of the fluid in the lubrication gap [36, 32], the formation of a tribofilm on the workpiece surface [32, 39], the influence of the cutting speed on the process [27], the thermal balance of the system, and the temperature field in the contact zone [36, 27]. Also, the reproducibility of cutting simulations was investigated [38].

This chapter is organized as follows: First, the simulation scenarios, the molecular models, as well as the observables used for characterizing the system are introduced. Then, the results are presented and discussed, which includes mechanical properties, the workpiece deformation, lubrication and the formation of a tribofilm, thermal properties, and the evaluation of the reproducibility.

2 Methods

2.1 Simulation Scenario

The simulation scenario used in this work is depicted in Fig. 1. It consists of a workpiece, a (cutting) tool and, in the lubricated cases, of a fluid. This models the contact zone of a machining process, e.g. the tip of an abrasive particle in micro grinding or an asperity contact. In the lubricated simulations, the tool was fully submersed in the fluid. In the dry cases, the tool was in a vacuum. The workpiece surface is in the x - y plane.

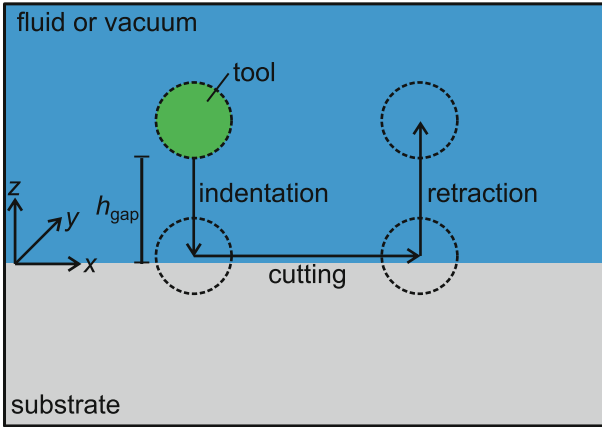


Fig. 1. Sketch of the simulation scenario. The scenario consists of a workpiece (grey), a tool (green), and a fluid or vacuum (blue).

The simulation box had periodic boundary conditions in x - and y -direction. The fluid was confined in the box by a soft repulsive wall at the top. The workpiece was locked in position by prescribing the at least three atom layers at the bottom of the box. Dissipated heat is removed from the system by imposing the initial system temperature (specified below for the different systems) to at least four atom layers above the fixed layer. In the course of the simulation, the tool carries out three consecutive movements: the indentation (negative z -direction), the cutting (positive x -direction), and the retraction (positive z -direction). Hence, the movement of the tool is predefined. Three different tool shapes were used: a sphere [27, 32], a spherical cap [39], and a cylinder [36, 38]. In the latter case, a quasi-2D scenario was considered. Moreover, different cutting gaps h_{gap} were considered for the cutting, cf. Figure 1. The simulations contained up to 9.2×10^6 particles per simulation. For the model system simulations, 5.43×10^6 particles were used in the simulations: 3.65×10^6 for the workpiece, 7.9×10^5 for the tool, and 1.78×10^6 for the fluid. For the real substance simulations, at least 8×10^5 particles were used for the workpiece, 7×10^5 for the tool, and 8.68×10^5 for the fluid. The molecular simulation software LAMMPS [24] was used for the simulations. Details on the simulation scenario can be found in Refs. [36, 27, 32, 39, 38].

2.2 Molecular Model

Simulations were carried out using a simplified model system as well as a real substance system, which are briefly introduced in the following. Details on the model system simulations are given in Refs. [36, 27, 38]. Details on the real substance systems in Refs. [32, 39].

2.2.1 Model Systems

The Lennard-Jones truncated and shifted (LJTS) model system is a generic and simplified system. Yet, this provides a reasonable representation of a real substances as the basis molecular interactions, i.e. repulsive and dispersive, are captured [35, 12, 44]. Hence, the simulations with the LJTS model system do not aim to model a specific real cutting process but to investigate general mechanisms of cutting processes and the influence of molecular interaction parameters. Despite its simplicity, the LJTS system provides a physically robustness model backbone and is, at the same time, computationally relatively cheap. In the presented model system, all occurring interactions were modelled by the LJTS potential (cf. Eq. 2.1).

$$u_{LJ}(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \text{ and} \quad (2.1)$$

$$u_{LJTS}(r) = \begin{cases} u_{LJ}(r) - u_{LJ}(r_c) & r \leq r_c \\ 0 & r > r_c \end{cases} \text{ with } r_c = 2.5\sigma$$

In Eq. (2.1), u_{LJ} indicates the full Lennard-Jones potential. For the LJTS potential, interactions are truncated at r_c and the potential energy u is shifted such that no discontinuity appears at the truncation radius. Each component (workpiece, fluid, and tool) has two molecular interaction parameters: the energy parameter ε and the size parameter σ . The size parameter σ as well as the particle mass m of all components were the same in all cases. The solid-solid interactions between the workpiece and the tool were described by the LJTS potential with a cut-off radius of $r_{\text{cut}} = 2^{1/6}\sigma$ such that they only interact repulsively. The workpiece energy parameter was chosen to represent iron [12] and the fluid energy parameter was chosen to represent methane [44]. All quantities for the LJTS model systems are given in reduced units (cf. Table 1) with respect to the fluid particle interaction parameters ε_F and σ_F . The solid-fluid interaction energy was systematically varied in the range $0 \leq \varepsilon_{SF}^* \leq 1.7$ to study its influence on the cutting process. The initial temperature was $T^* = 0.8$ and the initial pressure was $p^* = 0.014$.

2.2.2 Real Substance Systems

In the real substance simulations, the workpiece was modeled as a single crystal iron block, the tool was modeled as a diamond single crystal with a spherical tip shape, and the fluid was either methane or decane [32, 39]. The iron workpiece was described by an embedded atom model (EAM) [21]. The fluid was either modelled as methane by a BZS force field [44, 43] or as n-decane by the TraPPE force field [22], which provide an excellent description of the fluid bulk phase properties [29]. The diamond tool was modelled by a Tersoff potential [41]. For methane, the initial temperature was either 100 K (for simulations with a spherical indenter) or 130 K (for simulations with a spherical cap indenter). The initial pressure was 0.1 MPa and 50 MPa, respectively.

Table 1. Definition of physical quantities in reduced units. Reduced quantities are marked by (*). The Boltzmann constant is indicated as k_B .

Length	$L^* = L/\sigma_F$
Temperature	$T^* = T/(\epsilon_F/k_B)$
Force	$F^* = F/(\epsilon_F/\sigma_F)$
Time	$t^* = t/(\sigma_F\sqrt{m_F/\epsilon_F})$
Velocity	$v^* = v/\sqrt{\epsilon_F/m_F}$
Energy	$E^* = E/\epsilon_F$

2.3 Definition of Observables

Different quantities were computed from the simulation trajectories, which are briefly introduced in the following. The forces on the tool in tangential (x) and normal (y) direction, F_t and F_n , respectively, were calculated as the sum of all forces acting on the particles of the tool. The forces were calculated every 1000 timesteps. Mean values have been calculated during the cutting phase in the stationary part of the process. The coefficient of friction is defined as $\mu = F_t/F_n$. The coefficient of friction was calculated by the mean values of the forces from the stationary cutting phase. The internal energy of the fluid U_F and the workpiece U_S were calculated as the sum of the interaction energies between all respective particles. They were also sampled every 1000 timesteps. The energy dissipated by the thermostat in the substrate ΔU_{thermo} was computed as the energy difference after and before the thermostatization in each time step. The following quantities were calculated based on the configurational data of the particles that were written out at least every 10^4 timesteps. The number of fluid particles in the gap between the tool and the substrate were computed as N_{gap} . The gap was geometrically defined as depicted in Fig. 2 as the volume between the tool and the workpiece surface in front of the tool center and below the undeformed surface height. The surfaces were analyzed using the *alpha shape* algorithm [7]. Based on the calculated workpiece surface, the number of fluid particles below the surface that form a tribolayer were computed as N_{tribo} . The temperature profile in the x - z plane was sampled by averaging the per-atom temperature binwise. The bins are defined as depicted in Fig. 2. An estimation of the statistical uncertainty and significance of the observations is possible by the separate reproducibility study [38]. Details on the definition and sampling of the observables are given in Refs. [36, 27, 32, 39].

3 Results

3.1 Mechanical Properties

Figure 3. Shows the time evolution of the tangential and the normal force in cutting simulations for a dry case and a lubricated case. During the indentation, the normal force increases drastically when the tool penetrates into the workpiece and causes elastic and plastic deformation. In that phase, the tangential force fluctuates around $F_t = 0$. In the

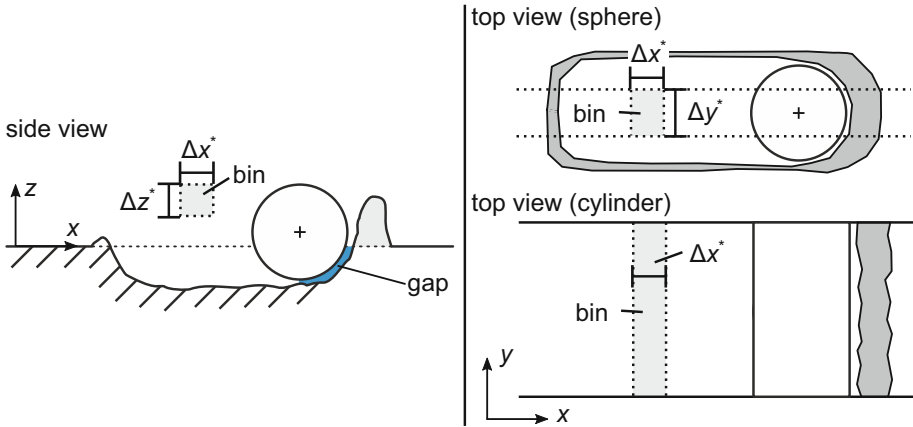


Fig. 2. Sketch illustrating the definition of observables. Left: Side view with the gap between the tool and the substrate and the bin to sample the temperature in x - y plane. Right: Top view with the bin to sample the temperature profile in x - y plane for the case of a spherical (top) and a cylindrical tool (bottom).

cutting phase, the normal force decreases and the tangential force increases until a steady state is reached. During the retraction, the both forces decay to zero.

Overall, the results from the dry and lubricated case are similar. Yet, the normal force on the tool is slightly affected by the cutting fluid during the indentation and the starting phase of the cutting. The peaks observed during the indentation in the dry case (caused by dislocation movement) are damped by the presence of the cutting fluid molecules in the gap. During the indentation, the vast majority of fluid particles is squeezed out of the gap. During the starting phase of the cutting, until a steady state is reached, the tangential force is slightly increased in the lubricated case compared to the dry case, which is due to an effective enlargement of the tool due to adsorbed fluid particles [32], i.e. the tool causes more elastic and plastic deformation of the workpiece in the lubricated cases. The coefficient of friction increases strongly in the starting phase of the cutting. In the starting phase, the lubricated simulations yield slightly lower coefficients of friction compared to the dry simulations due to lubricant molecules remaining in the gap between the tool and the substrate. In the stationary phase, the coefficient of friction is very similar in the dry and the lubricated case with values between 0.4 and 0.6. Since the differences between the dry and lubricated case are small and might in general be within the scattering of the results, the reproducibility of the findings discussed here was studied (and confirmed) using the model system, cf. Sect. 3.4.

The influence of the solid-fluid interaction energy ε_{SF}^* on the cutting process was systematically investigated using the LJTS model system [36]. The results are shown in Fig. 4. In the starting phase of the cutting process, the coefficient of friction in the lubricated cases is reduced by about 25% compared to the dry case. This is due to an increased normal force and a slightly decreased tangential force in the starting phase [36]. In the stationary phase, the coefficient of friction is increased in the lubricated case compared to the dry case by approximately 15%, which is due to individually fluid

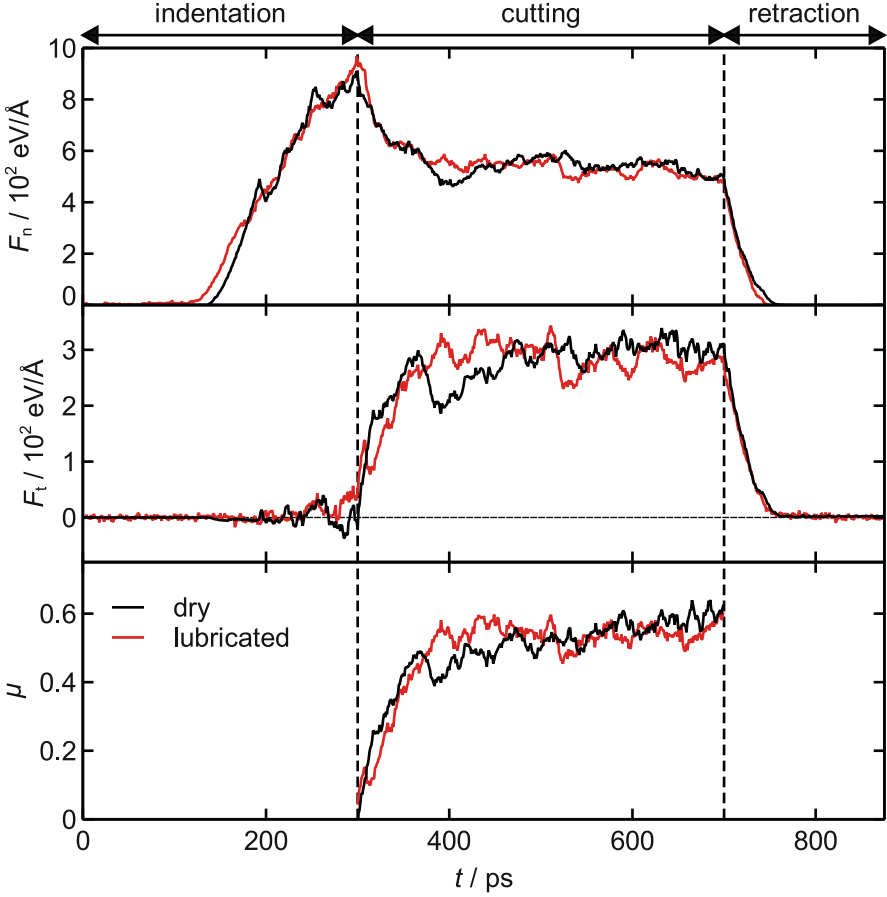


Fig. 3. Normal (top) and tangential (bottom) forces on the tool as a function of time for a dry and a lubricated simulation [32]. The tool had a spherical shape. The temperature was $T = 100$ K. The workpiece was an iron single crystal, the tool was a diamond, and the fluid was methane.

particles being imprinted into the workpiece surface. Interestingly, these findings do not depend on the solid-fluid interaction energy. The coefficient of friction is reduced in the starting phase due to fluid molecules remaining in the gap and effectively increasing the tool size. These fluid molecules are squeezed out mostly with ongoing cutting process. The squeeze out process is discussed in detail in Sect. 3.3.

Figure 5. Shows the results for the influence of the cutting speed on the coefficient of friction. For both cases (dry and lubricated), no significant influence of the cutting speed on the coefficient of friction is observed in the considered velocity range. For the smallest considered cutting speed $v^* = 0.66$, the coefficient of friction is nearly the same for the dry and the lubricated simulations with $\mu^* \approx 0.85$. For the velocities $0.1 < v^* < 0.3$, the lubricated simulations yield smaller values for the coefficient of friction compared to the dry simulations. These differences are probably within the uncertainty of the data. This is supported by the result for the highest considered velocity $v^* = 0.332$, which

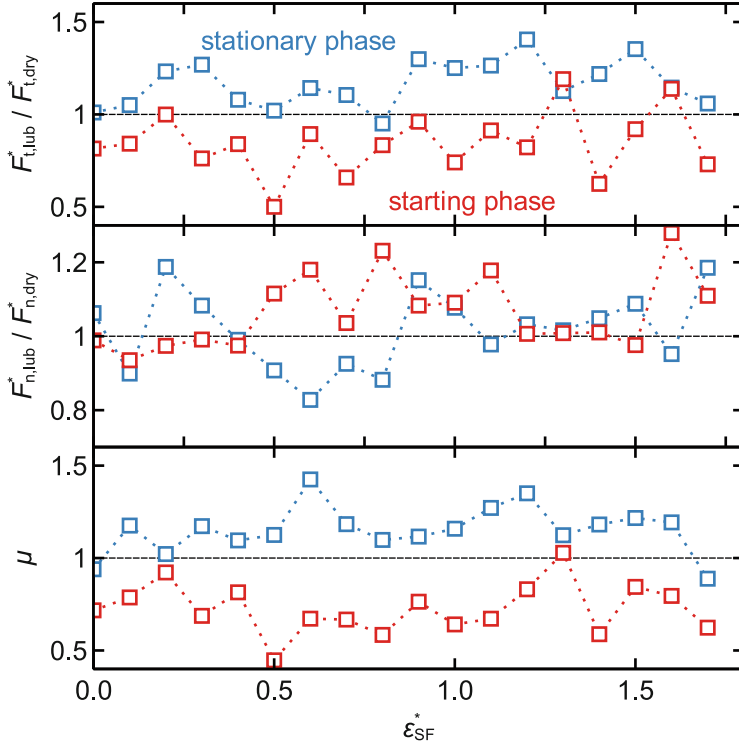


Fig. 4. Tangential force (top), normal force (middle), and coefficient of friction (bottom) of the lubricated simulations related to the dry simulation as function of the solid-fluid interaction ε_{SF}^* [36]. The tool had a cylindrical shape. The temperature was $T^* = 0.8$. The workpiece, the tool, and the fluid were modeled by the LJTS potential. Mean values for the starting phase (red, $142 < t^* < 335$) as well as the stationary phase (blue, $335 < t^* < 625$).

show the opposite trend. Using the potential parameters for methane and iron [12, 44] for the fluid and workpiece, respectively, the cutting speed range corresponds to 20 - 100 m/s in SI units, which is typical for cutting and grinding processes [20, 5]. In the literature, relative velocities between two solid bodies up to 400 m/s were considered using molecular simulation (which is not representative for common manufacturing cutting processes). Nevertheless, in this high-speed regime, the coefficient of friction was reported to decrease with increasing velocity [23, 46].

Using the real substance system simulation setup, the influence of the cutting depth, i.e. the z -position of the tool with respect to the workpiece surface, was systematically investigated [39]. Here, also configurations with no direct contact between tool and substrate were considered, i.e. hydrodynamic lubrication (HL). In Fig. 6, the forces on the tool as well as the coefficients of friction are shown as function of the cutting depth h . Results are given for decane as fluid. Three different lubrication regimes can be identified for different cutting depth: hydrodynamic lubrication (HL), mixed lubrication (ML), and boundary lubrication (BL). The normal and tangential force on the tool increase with increasing cutting depth as expected. The normal forces are larger than the tangential

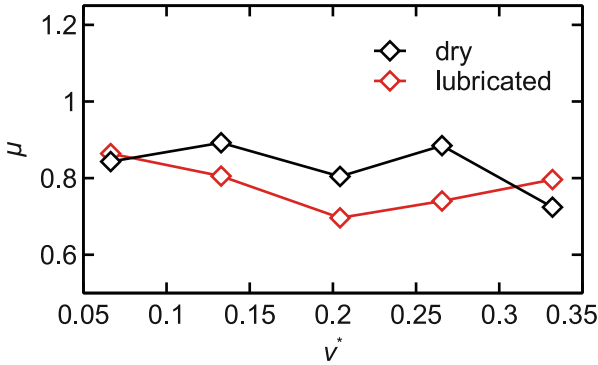


Fig. 5. Coefficient of friction μ as a function of the tool velocity v^* for a dry and lubricated cases [27]. The tool had a spherical shape. The temperature was $T^* = 0.8$. The workpiece, the tool, and the fluid were modeled by the LJTS potential.

forces in general. The coefficient of friction behaves differently in the three regimes. In the HL regime, the coefficient of friction is lowest – as expected. Here, a stable fluid film separates the two solids and leads to a good lubrication with small values of the coefficient of friction. In the ML regime, the coefficient of friction increases with increasing cutting depth as the normal force strongly increases due to the direct contact between the tool and the workpiece, which is transferred via the thin lubrication film. The coefficient of friction reaches a maximum of $\mu \approx 0.21$ at the border between the ML and BL regime. For larger cutting depth (BL regime), the coefficient of friction decreases with increasing cutting depth. The behavior in the BL regime is mainly determined by the formation of a tribofilm, the squeeze-out and the resistance of the lubrication film. Therefore, the tangential force increases more strongly compared to the normal force, which leads to a decrease of the coefficient of friction.

3.2 Workpiece Deformation

In the following, phenomena related to the surface of the workpiece and to the formation of dislocations in the workpiece are discussed. Figure 7 shows the results for the total dislocation length as a function of the simulation time for a dry and a lubricated case. Overall, the results for the dry and the lubricated case are similar. In the indentation phase, the presence of the cutting fluid leads to a slightly earlier formation of dislocations compared to the dry simulation, which was also confirmed by replica simulations of a model systems in an earlier work of our group [38]. This is probably due to fluid adsorption layers on both the workpiece and the tool surface that effectively increases the size of the tool and lead to an earlier starting of elastic and plastic deformation on the workpiece. During the cutting phase, the dislocation length slightly increases in the dry case and the lubricated case. The presence of the fluid has only minor effects on the dislocation behavior – also considering the statistical uncertainties of the data [38]. After the retraction, an annihilation of some of the dislocations can be observed as the total dislocation length decreases.

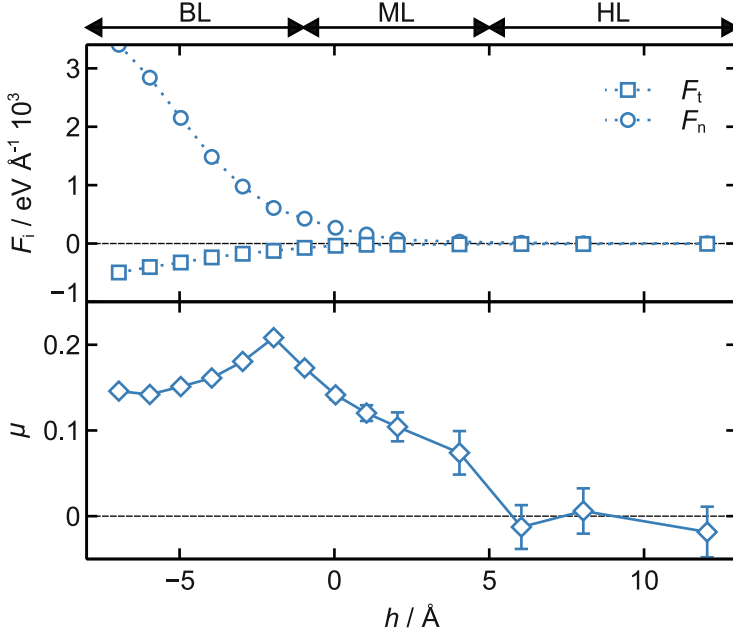


Fig. 6. Normal and tangential forces on the tool (top) and coefficient of friction (bottom) as a function of the cutting depth for simulations with decane [39]. The tool was a spherical cap. The temperature was $T = 350$ K. The workpiece was an iron single crystal, the tool was a diamond, and the fluid was decane. Three different regimes were distinguished: boundary lubrication (BL), mixed lubrication (ML), and hydrodynamic lubrication (HL). The statistical uncertainties were estimated from the fluctuation of block average values in the quasi-stationary cutting phase.

Figure 8 shows the deformed substrate surface at the end of the cutting process. Results are shown for two different cutting depths for both methane and decane as fluid. For a cutting depth of $h = -2\text{\AA}$, the cutting process roughens the surface over the entire cutting length, which is mostly due to the formation of a tribofilm.

No distinct chip formation is observed for $h = -2\text{\AA}$, cf. Fig. 8. A distinct chip formation is obtained for $h = -6\text{\AA}$, cf. Fig. 8 (bottom). The chip forms primarily at the sides of the tool which is built-up by the workpiece atoms that are thrust aside of the tool. Comparing the methane results with the decane results, the chip is more pronounced and the atoms at the workpiece surface are less disordered in the methane case. This is due to the different characteristics of the adsorption layers of methane and decane [39] including the particles trapped in the gap between the tool and the substrate.

3.3 Lubrication and Formation of Tribofilm

The number of fluid particles trapped in the gap between the tool and the workpiece (cf. Fig. 2) were computed at the end of the indentation phase. These results are shown as a function of the solid-fluid interaction in Fig. 9. For the case of no attractive interactions between the solid and the fluid particles, the number of particles in the gap N_{gap} at the

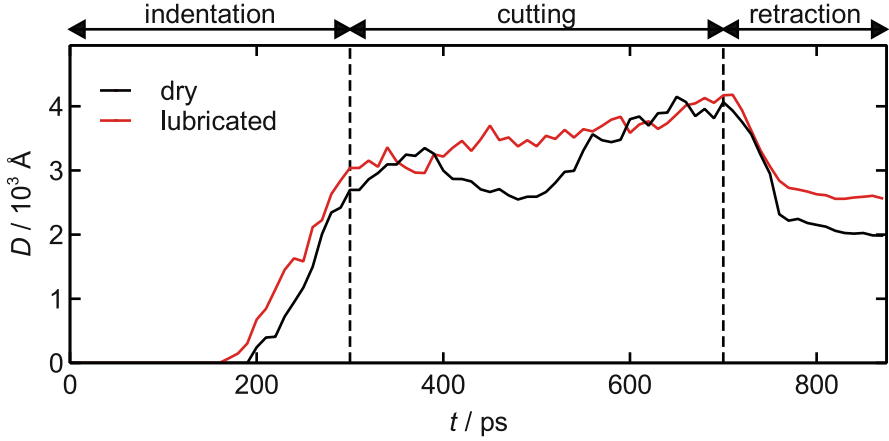


Fig. 7. Dislocation length in the workpiece as a function of time for a dry and a lubricated simulation [32]. The tool had a spherical shape. The temperature was $T = 100$ K. The workpiece was an iron single crystal, the tool was a diamond with a spherical tip shape, and the fluid was methane. The dislocation analysis was carried out with the DXA algorithm [40].

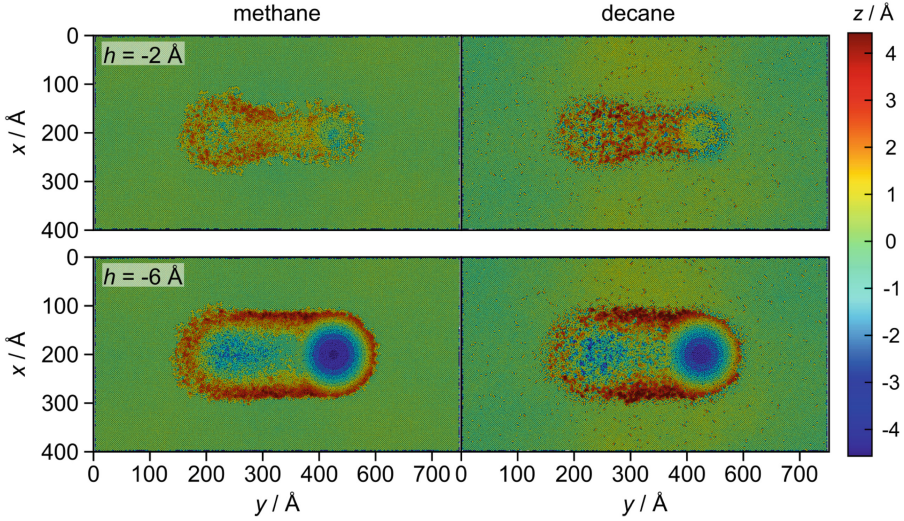


Fig. 8. Top view on the workpiece surface at the end of the cutting phase for the cutting depths $h = -2, -6$ Å (top to bottom) [39]. Results are shown for simulations with methane (left) and decane (right) as fluids. The tool was a spherical cap. The workpiece was an iron single crystal and the tool was a diamond. The visualizations were created using Paraview [15].

end of the indentation is lowest and close to zero. With increasing solid-fluid interaction energy, more particles remain trapped in the gap until a steady plateau is reached for approximately $\varepsilon_{SF}^* \approx 0.75$. For larger values, N_{gap} stays approximately constant. Interestingly, this behavior is in line with the contact angle behavior of the studied LJTS

system [4], i.e. total wetting is reached at approximately $\varepsilon_{SF}^* \approx 0.75$. This means the number of particles increases with decreasing contact angle until total wetting is reached.

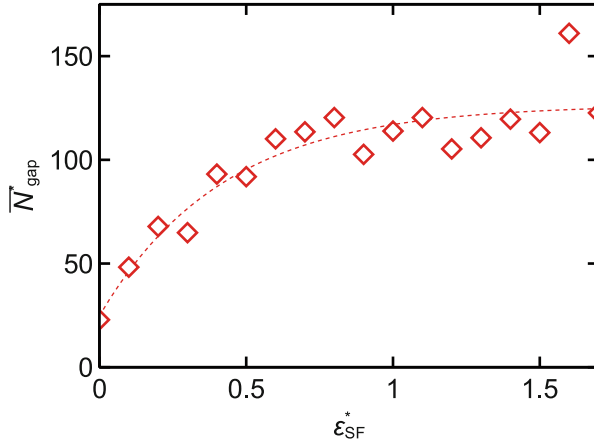


Fig. 9. Number of fluid particles in the gap between the tool and the workpiece $\overline{N}_{gap}^*$ (cf. Fig. 2) as function of the solid-fluid interaction energy ε_{SF}^* [36]. The tool had a cylindrical shape. The temperature was $T^* = 0.8$. The workpiece, the tool, and the fluid were modeled by the LJTS potential. The dashed line is an empirical correlation of the form $\overline{N}_{gap}^* = 126.5 - 101.7e^{-\varepsilon_{SF}^*/0.422}$.

The properties of the surface are strongly influenced by single fluid molecules that are imprinted into the workpiece surface. This is observed for both the methane as well as the decane case. Yet, both systems show different characteristics due to the different molecular shape of the fluid molecules. A screenshot of each system is shown in Fig. 10. The imprinted fluid molecules can be interpreted as a tribofilm that forms in the upper part of the workpiece near the surface due to the extreme load. In the case of methane, the tribofilm is mainly build-up by methane atoms occupying regular lattice sites of the iron crystal. The overall lattice structure of the workpiece remains undamaged in this case. Due to decane being a long linear chain molecule, the workpiece lattice structure is significantly broken up in the decane case. Decane molecules are also imprinted into the substrate surface, but the imprinted molecules destroy the regular lattice and cause an unstructured formation of the upper atom layers of the workpiece.

The formation of a tribofilm is further analyzed in Fig. 11, which shows the number of fluid particles imprinted in the substrate surface N_{tribo} as a function of the z -coordinate for three different cutting depths.

The formation of the tribofilm is mainly observed at large cutting depth as the number of imprinted fluid particles is significantly lower. For both studied fluids, the number of fluid particles is largest for $z \approx -2\text{\AA}$ and the number decreases with decreasing z . For methane, the imprinted sites reach depths of up to $z = -12\text{\AA}$. The decane sites only reach depths of up to $z = -9\text{\AA}$. The different characteristics observed in the screenshots (cf. Fig. 10) can be confirmed by the histograms shown in Fig. 11. The methane particles are accumulated at specific depths, i.e. distinct peaks forming in the histogram. This is due to the methane particles occupying regular lattice sites of the workpiece lattice.

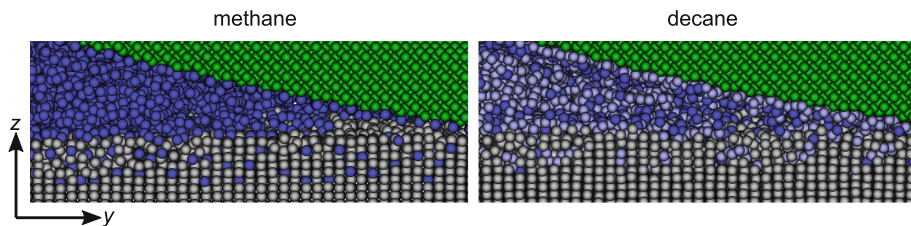


Fig. 10. Screenshots of the rear side of the contact zone (tool moves to the right) at cutting depth $h = -6\text{Å}$ [39]. The tool was a spherical cap. The workpiece was an iron single crystal, the tool was a diamond, and the fluid was methane (left) or decane (right). Green particles indicate tool particles, grey particles the workpiece particles, dark blue CH_4 (left) or CH_3 (right) sites (end group of decane), and light blue CH_2 sites (middle group of decane).

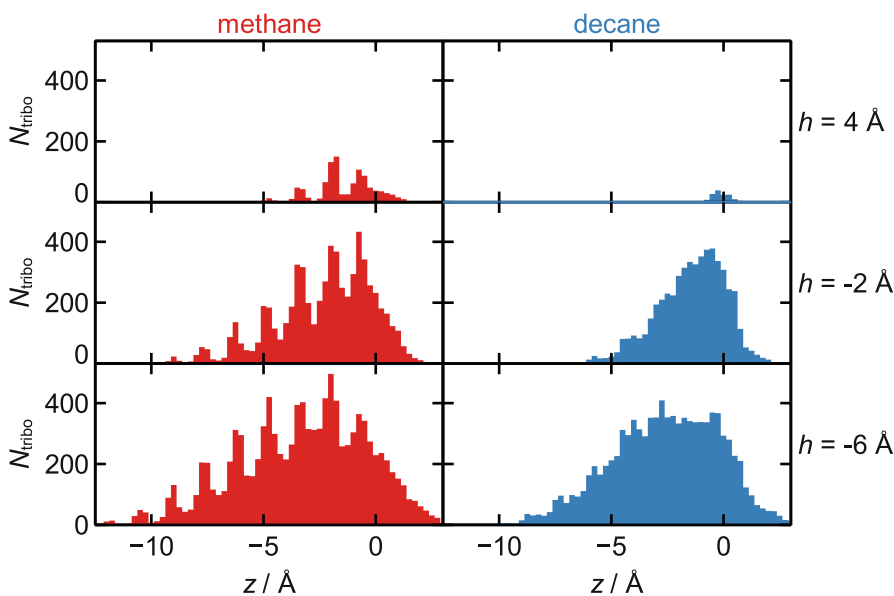


Fig. 11. Histograms of fluid particles imprinted in the workpiece surface N_{tribo} as a function of the z -coordinate [39]. Results for $h = 4, -2, -6\text{Å}$. The tool was a spherical cap. The workpiece was an iron single crystal, the tool was a diamond, and the fluid was methane (left) or decane (right).

For the decane simulations, these peaks cannot be observed which is in line with the unstructured tribofilm observed in Fig. 10.

3.4 Thermal Properties

Thermal properties of a cutting process such as the temperature in the contact zone and the heat flux absorbed by the workpiece, are crucial for the product quality and the manufacturing process. The MD simulations carried out in this work were evaluated in detail

regarding the thermal properties. Figure 12 shows the spatial temperature distribution in the $x^* - y^*$ plane by snapshots at a cutting length of $L^* = 77$.

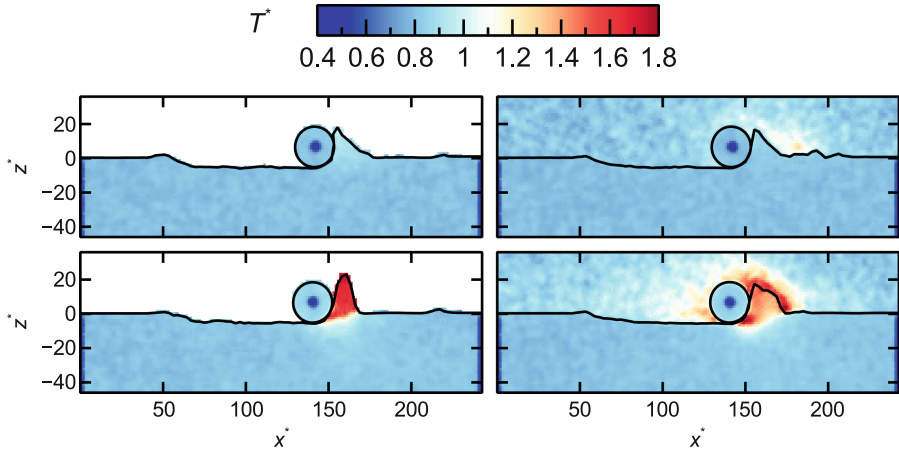


Fig. 12. Temperature profile in the $x^* - y^*$ plane at the cutting length $L^* = 77$ for dry (left) and lubricated (right) simulations [27]. Results shown for two different velocities, $v^* = 0.066$ (top) and $v^* = 0.332$ (bottom). The tool had a spherical shape. The bulk temperature was $T^* = 0.8$. The workpiece, the tool, and the fluid were modeled by the LJTS potential.

The evaluation procedure is depicted in Fig. 2. Simulation results for two different cutting speeds, $v^* = 0.066$ and $v^* = 0.332$, are shown. Results from a dry case are compared to the results from a lubricated case. The temperature increases for both cases with increasing tool velocity. In the dry simulation, the temperature increases mainly in the chip, i.e. the energy dissipates in the direct vicinity of the contact zone – as expected. From the chip, the heat is transported to the bulk of the substrate in the dry case. In the simulation scenario, the tool is thermostatted which is why the temperature in the tool keeps constant. If a fluid is present, the increase of the temperature in the contact zone is reduced as the heat is also transported into the fluid. Therefore, the temperature of the cutting fluid near the contact zone is increased compared to the bulk fluid temperature. Hence, the fluid has important cooling capabilities.

In Fig. 13, the results for the energy balance of the system are shown. The energy balance includes all sources and sinks of the system. Energy is added to the system by the work done by the tool. Energy is removed from the system by a thermostat in the workpiece (cf. Fig. 13). In the cutting simulations, the thermostat acts as a heat sink and removes dissipated energy from the system such that a quasi-stationary state is established. The energy which is not removed by the thermostat heats up the substrate and (if present) the fluid, i.e. their internal energy increases. The change of the internal energy of the workpiece U_W and the fluid U_F , energy removed by the thermostat ΔU_{thermo} , and the work done by the tool W_T are shown in Fig. 13 as a function of time. Therein, U_W and U_F indicate the changes of the total energy (kinetic and potential) of the workpiece and fluid particles, respectively. The energy removed from the system ΔU_{thermo} was computed from the rescaled kinetic energy imposed by the thermostat. The work done

by the tool W_T was computed from the integral of the total force (in moving direction) during the process. The fluid strongly influences the energy balance of the process.

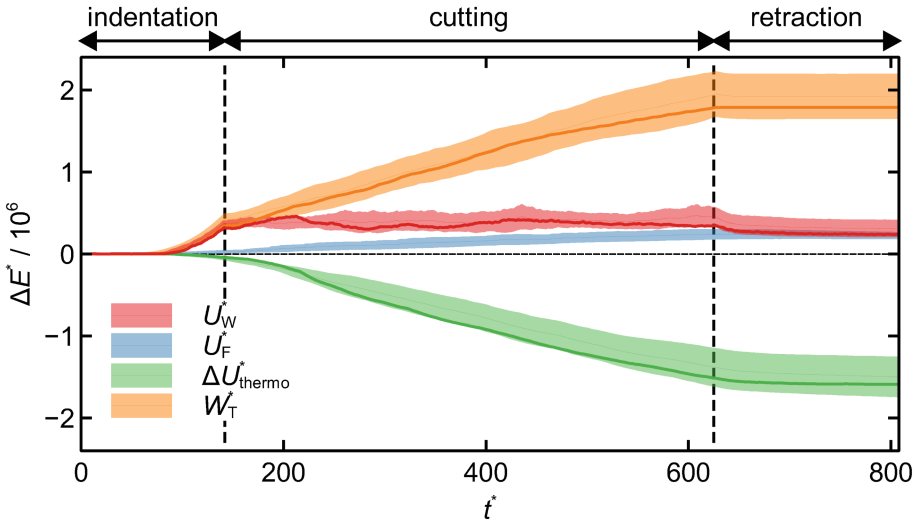


Fig. 13. Energy balance of the system including internal energy changes of the workpiece U_W and the fluid U_F , energy removed by the thermostat ΔU_{thermo} , and the work done by the tool W_T [36]. The shaded areas include all lubricated simulation cases with different solid-fluid interactions energies. The solid lines represent the dry simulation case. The tool had a cylindrical shape. The initial temperature was $T^* = 0.8$. The workpiece, the tool, and the fluid were modeled by the LJTS potential.

The heat removed by the thermostat as well as the change of the internal energy of the substrate is reduced up to 20% by the presence of a fluid. This cooling effect depends on the solid-fluid interaction energy [36]. The fluid reduces the friction during the cutting phase, and part of the dissipated energy in the contact zone heats up the fluid, which directly cools the contact zone. Nevertheless, the main part of the energy added to the system by the cutting process is dissipated. The energy dissipated is significantly larger than energy required for the defect generation and plastic deformation.

3.5 Reproducibility

The statistical uncertainties and the reproducibility of the simulation method was assessed using a set of eight replicas. The single simulations of the set only differ in their initial velocities that are assigned before the equilibration of the simulation box. Based on the eight replica simulations, the standard deviation σ was calculated for several observables. In Fig. 14, the results for the normal force are shown. The time evolution of the normal force agrees in general with the results given in Fig. 3. The higher normal force in the case with a fluid compared to the dry case is confirmed by these results. The standard deviation of the normal force among the replica simulations is relatively small in the indentation phase.

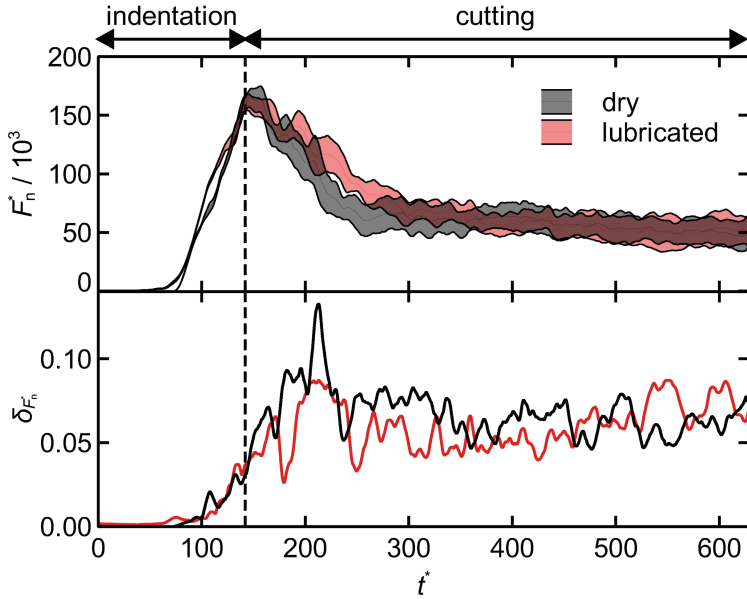


Fig. 14. Normal force on the tool as a function of time for the dry and the lubricated case (top) and the corresponding instantaneous standard deviation (bottom) [38]. The shaded area includes the entire range of the results of all eight replica simulations. The tool had a cylindrical shape. The temperature was $T^* = 0.8$. The workpiece, the tool, and the fluid were modeled by the LJTS potential.

The standard deviation increases with progressing indentation. In the starting phase of the cutting (cf. Sect. 3.1), the lubricated simulations show significantly higher statistical uncertainties. At the beginning of the stationary phase ($t^* \approx 300$), the normal forces in the dry and the lubricated simulations agree within the scattering of the replica sets. The standard deviation is slightly higher in the dry simulations in the starting phase of the cutting compared to the lubricated simulations.

In Fig. 15, the coefficient of friction calculated from the eight replicas is shown with its corresponding standard deviation. In the starting phase ($t^* < 300$), the coefficient of friction of the dry simulations is significantly larger compared to the simulations with a fluid. The difference exceeds the scattering of the replica sets, which indicates that the differences between a lubricated and a dry case in the starting phase are significant. The coefficient of friction is reduced in the lubricated case in the starting phase of the cutting due to fluid particles trapped in the gap between tool and the workpiece (cf. Sect. 3.3). Until the fluids are squeezed out of the gap, the tool experiences a larger normal force, which decreases the coefficient of friction in a lubricated case compared to a dry case. In the stationary phase of the cutting process, the coefficient of friction is slightly increased in the lubricated case, which is due to individual fluid particles being imprinted into the workpiece surface, which requires additional work done by the tool in the lubricated case. In general, no systematic differences in the reproducibility of dry and lubricated simulations were found. Moreover, the time dependency of the standard deviation for

the normal force and the coefficient of friction indicate that no differences between the simulations of a replica build up with ongoing process.

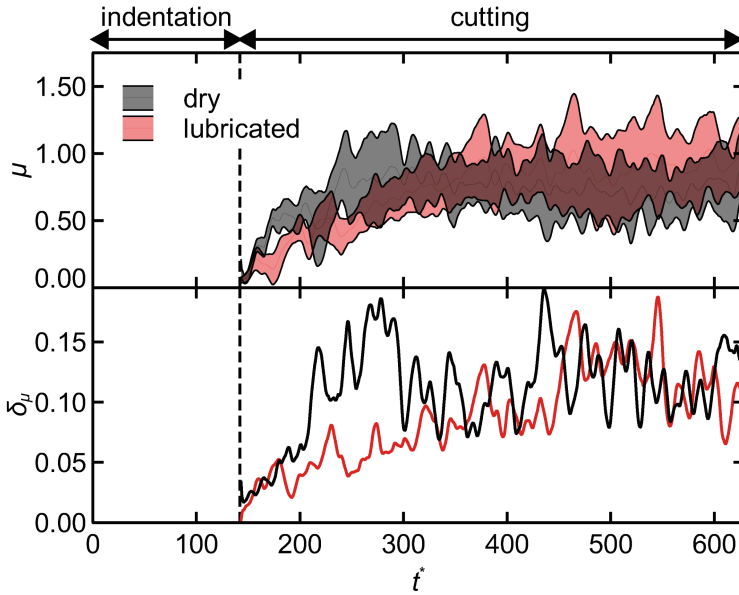


Fig. 15. Coefficient of friction as a function of time for the dry and the lubricated case (top) and the corresponding instantaneous standard deviation (bottom) [38]. The shaded area includes the entire range of the results of all eight replica simulations. The tool had a cylindrical shape. The temperature was $T^* = 0.8$. The workpiece, the tool, and the fluid were modeled by the LJTS potential.

4 Conclusions

In this work, the influence of lubrication on the contact zone of cutting processes was studied on the atomistic scale using classical MD simulation. Thereby, new insights were obtained on the fundamental mechanisms of lubrication and cooling provided by the presence of cutting fluids. Different simulations scenarios were used including model systems as well as real substance systems. The mechanical properties of the contact were studied in means of the normal and tangential force as well as the coefficient of friction. It was found that the presence of a fluid has an important influence in the starting phase of the atomistic cutting process, i.e. decreases the coefficient of friction, which is due to fluid molecules trapped in the gap between the workpiece and the tool. The influence of the cutting depth on the cutting process was investigated using two different fluids: methane and decane. Based on the results, three different lubrication regimes were identified for different cutting depths: the hydrodynamic lubrication regime for very small cutting depths, the mixed lubrication regime for cutting depths that correspond approximately to the size of fluid molecules, and the boundary lubrication regime cutting for cutting

depths that yield significant elastic and plastic deformation of the workpiece. Within these different regimes, the coefficient of friction shows different characteristics.

The presence of a fluid has important thermal effects on the atomistic cutting process, i.e. it is found to reduce the maximum temperature in the contact zone and reduce the heat impact of the workpiece. The heat absorbed by the workpiece is reduced by up to 20% by the presence of a fluid lubricant. For future for, the simulation scenario should be refined, e.g. considering a rough surface topography, such that the reality of tribological contact processes is captured in more detail.

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