The Influence of Lubrication and the Solid-Fluid Interaction on Thermodynamic Properties in a Nanoscopic Scratching Process

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Abstract

Liquid lubricants play an important role in contact processes, e.g. they reduce friction and cool the contact zone. To gain better understanding of the influence of lubrication on the nanoscale, both dry and lubricated scratching processes in a model system are compared in the present work using molecular dynamics simulations. The entire range between total dewetting and total wetting is investigated by tuning the solid-fluid interaction energy. The investigated scratching process consists of three sequential movements: A cylindrical indenter penetrates an initially flat substrate, then scratches in lateral direction, and is finally retracted out of the contact with the substrate. The indenter is fully submersed in the fluid in the lubricated cases. The substrate, the indenter, and the fluid are described by suitably parametrized Lennard-Jones model potentials. The presence of the lubricant is found to have a significant influence on the friction and on the energy balance of the process. The thermodynamic properties of the lubricant are evaluated in detail. A correlation of the simulation results for the profiles of the temperature, density, and pressure of the fluid in the vicinity of the

chip is developed. The work done by the indenter is found to mainly dissipate and thereby heat up the substrate and eventually the fluid. Only a minor part of the work causes plastic deformation of the substrate.

Introduction

Tribological processes are of fundamental importance in many technical applications, but also in nature. It is well known that using liquid lubricants entails two main advantages: the reduction of friction and the cooling of the contact zone. However, the origin of these phenomena is yet not fully understood on an atomistic level.^{1–4} The region in which two solid bodies interact directly under the influence of a lubricant is extremely small and practically inaccessible for experimental studies, so that only little is known on the phenomena in that zone. Molecular simulation provides an attractive tool to elucidate such processes.^{5–11} The results from molecular simulations of a given scenario are obtained by solving Newton’s equation of motion and depend solely on the force field that describes the molecular interactions. If these interactions are reasonably described, the method has strong predictive capabilities.^{12,13}

There are many studies on dry nanoindentation and scratching processes see e.g. refs.^{2,14–17} For example, the influence of the shape of the indenter,^{18,19} substrate materials,^{5,20,21} indentation depth,²² cutting direction in relation to the lattice orientation,²³ grain boundaries,²⁴ surface roughness,²⁵ alloys,²⁶ coatings,²⁷ and temperature²⁸ were investigated. Also shear flow friction simulations where two solid bodies are separated by a fluid have been extensively investigated in the literature, e.g.^{29–39,39–45}

Lubricated scratching processes where two solid bodies are in direct contact under the influence of a fluid, on the other hand, have not been investigated as systematically. Results on the influence of the chain length of the lubricant molecules,^{46,47} the surface roughness,^{48,49} adsorbates,^{6,50–58} the squeeze-out of lubricant molecules,^{9,48,59} and the surface chemistry^{60,61} have been reported in the literature. In most of these studies, lubrication was only considered by single adsorbed layers of fluid molecules on the substrate surface in the simulation, while studies in which the contact is

truly immersed in a liquid are still rare.^{7,9,62,63} Also, small systems with state of the art ab initio MD^{64–67} have been reported recently. None of these studies systematically addresses the question of the influence of the lubricant on the thermal balance of the system, i.e. its cooling capability or the behavior of the fluid due to the dissipation in the vicinity of the contact zone.

Also, to the best of our knowledge, no systematic study has been performed yet that addresses the influence of the solid-fluid interaction energy on nanoscopic scratching processes where two solid bodies are in direct plastically deforming contact and are fully immersed in a liquid. The solid-fluid interaction energy determines the adsorption and the wetting behavior of the lubricant on the solid surfaces.^{68–70} *Becker et al.*⁶⁸ have investigated liquid droplets on solid surfaces in Lennard-Jones systems and determined the influence of the solid-fluid interaction energy on the contact angle.

In the present study, we report on molecular dynamics simulations of a three-stage nanoscopic contact process consisting of indentation, scratching, and retraction of a cylindrical indenter on an initially atomistically flat single crystal substrate. All three components (substrate, indenter, and fluid) are described by the Lennard-Jones potential, which puts the present study in line with those from *Becker et al.*⁶⁸ The Lennard-Jones potential is often used in molecular physics as it is known to describe the thermodynamic properties of simple fluids very well^{12,68,71–76} and still gives a reasonable model for some solid crystals.^{77–79} The Lennard-Jones potential is computationally cheaper than more realistic EAM potentials,⁸⁰ and facilitates a systematic investigation of the influence of the solid-fluid interaction energy on the scratching process. The Lennard-Jones potential has been widely used for studying fundamentals in nano tribology, e.g. for the modeling of dispersive and repulsive interactions of simple spherically shaped fluid molecules^{7,9,31,32,37,81} as well as such interactions between chain molecules^{35,37,45–47,54}, the modeling of the solid-fluid interactions^{6,7,9,30,35,37,43,45–47,50,52,53,55}, and also the modeling of solid-solid interactions.^{9,62,63}

Nevertheless, the simplicity of the chosen model limits the applicability and transferability to real systems. Evidently, a Lennard-Jones sphere is not a good representative for oils and fats often used in cutting processes to reduce friction. Also, it is well accepted that the Lennard-Jones potential does not capture the plasticity and elasticity of real solid materials accurately. A further crude

simplification compared to a real system is that the substrate surface is atomistically flat and the substrate block is a single crystal without grain boundaries that are known to influence contact processes^{24,82}. Also, the negligence of surface chemistry effects is a strong simplification. Hence, the present work does not aim at modeling the cutting process of a certain real system, but instead at describing a simplified yet representative system in a generalized approach. This concept study of an idealized model provides insight in the mechanisms of a fully immersed cutting process on a nanoscale.

The focus of this work lies on the investigation of thermal effects in scratching processes, like grinding and polishing of microstructures.^{14,15,83,84} The cooling of both the workpiece and the tool, the overall energy balance as well as the local temperature are crucial process parameters in such machining processes,^{85–91} but often not accessible by experiments – especially the local temperature field. Models used to estimate and predict these process parameters in engineering applications, i.e. estimating the dissipation and the distribution of the heat in a machining process are mostly empirically motivated, cf.^{87,90,92,93} and little is known regarding the underlying molecular processes. Our work investigates the thermal and mechanical behavior of a simplified machining process and thereby contributes to a better understanding of high precision machining processes^{83,94} on the nanoscale.

Despite the simplicity of the model system, the results are also applicable to technical applications such as liquid methane in cryogenic pumps for LNG (liquid natural gas) processes^{95–98} and for the next generation of rocket engines^{99,100} or liquid nitrogen (N_2)¹⁰¹ as metal working fluid in cryogenic machining processes,^{102–104} as well as in pumps in air separation units^{105,106} for the production and purification of argon and nitrogen.

The article is organized in two parts: in the first part, the simulation method and scenario are introduced and the observed properties are defined. In the second part, the results of the replicated studies of the scenarios are presented and discussed.

Methods

Molecular Model

Fig. 1 shows the simulation setup, which consists of a cylindrical indenter (I), a substrate (S), and eventually in the lubricated cases, a fluid (F). All three components are modeled with the Lennard-Jones potential, which is truncated and shifted at $r_c = 2.5 \sigma$:

$$u_{\text{LJ}}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad \text{and} \quad (1)$$

$$u_{\text{LJTS}}(r) = \begin{cases} u_{\text{LJ}}(r) - u_{\text{LJ}}(r_c) & r \leq r_c \\ 0 & r > r_c, \end{cases} \quad (2)$$

with u_{LJ} being the full Lennard-Jones potential and u_{LJTS} the truncated and shifted potential. ϵ and σ are the energy and size parameter, respectively. The distance between two particles is r . The cut-off radius is $r_c = 2.5 \sigma$ throughout this work, except for the indenter-substrate (IS), which is kept purely repulsive by setting $r_c = 2^{1/6} \sigma$. This setting was also used in a case study in which the adsorption of the fluid on the indenter and the substrate was suppressed.

Throughout the present work, all physical properties are reduced¹² using the Lennard-Jones potential parameters of the fluid $\epsilon = \epsilon_{\text{F}}$, $\sigma = \sigma_{\text{F}}$, and the molecular mass M , as well as the Boltzmann constant k_{B} . The reduced properties are labeled with an asterisk, e.g. the temperature $T^* = T/(\epsilon/k_{\text{B}})$, the density $\rho^* = \rho/(1/\sigma^3)$, the pressure $p^* = p/(\epsilon/\sigma^3)$, the internal energy $U^* = U/\epsilon$, the work $W^* = W/\epsilon$, the heat $Q^* = Q/\epsilon$, the force $F^* = F/(\epsilon/\sigma)$, the time $\tau^* = \tau/(\sigma\sqrt{M/\epsilon})$, lengths and distances $s^* = s/\sigma$ (where s can be radius R , depth d , or dimensions x, y and z), the volume $V^* = V/\sigma^3$, and the velocity $v^* = v/\sqrt{\epsilon/M}$. The simulations were performed with the open-source code LAMMPS.¹⁰⁷

For convenience, the size parameter σ of the Lennard-Jones sites of the indenter, the substrate, and the fluid are identical. The same holds for the masses M . The dispersion energies ϵ are chosen so that the three components represent realistic materials. The dispersion energy of the fluid ϵ_{F} is chosen such that it describes methane employing the parameters proposed by *Vrabec et al.*⁷⁴

The dispersion energy of the substrate is adopted from *Halicioglu et al.*⁷⁹ such that it models iron energetically. The indenter is a rigid body, with its particles placed on a diamond lattice. The diamond lattice constant of the indenter is 1.55σ .

In the present study one dry simulation (no fluid present) is compared to 18 different lubricated cases. The latter ones differ only in the energy of the solid-fluid interaction. The solid-fluid interaction energy in each of the lubricated simulations is the same for the indenter-fluid (IF) and the substrate-fluid (SF) interaction and is denoted by a tilde $\tilde{\epsilon}^*$ throughout this work, i.e. $\tilde{\epsilon}^* = \epsilon_{\text{IF}}^* = \epsilon_{\text{SF}}^*$. The parameter of the solid-fluid interaction energy $\tilde{\epsilon}^*$ was varied between 0 and 1.7 with an increment of 0.1. For the simulation with $\tilde{\epsilon}^* = 0$, the fluid only exhibits repulsive interactions with the indenter and the substrate (employing the WCA potential,¹⁰⁸ which has $r_c = 2^{1/6} \sigma$). The 18 lubricated simulations cover the entire range of total wetting to dewetting.⁶⁸ *Becker et al.*⁶⁸ reported that total wetting in Lennard-Jones systems, i.e. a contact angle of 0° , is found for approximately $\tilde{\epsilon}^* \geq 0.75$ at approximately $T^* = 0.8$. The solid-fluid interaction energy $\tilde{\epsilon}^*$ is also directly related to the so called *slip length* at solid-fluid interfaces, as reported from shear flow friction simulations for a large number of real substances,^{32,34,35,37,109–112} and Lennard-Jones systems.^{31,33}

Table 1 summarizes choices that were made for the interactions in the form of a matrix of all three components (S, I, F) and their cross-interactions with respect to the dispersion energy of the fluid. The self interactions are denoted as the diagonal components, the cross-interactions as the off-diagonal components in Table 1.

Simulation Setup

The indenter carries out three sequential movements during the simulation, cf. Fig. 1: (i) indentation, during which the indenter penetrates into the substrate in $-z$ -direction normal to the unpenetrated substrate surface; (ii) scratching, during which the indenter moves laterally through the surface in $+y$ -direction, forming a groove; and (iii) retraction in $+z$ -direction, which brings the indenter out of the contact with the substrate. The indentation is carried out between $0 < \tau^* < 142$, the scratching between $142 < \tau^* < 625$, and the retraction between $625 < \tau^* < 809$.

The movement of the rigid indenter is fully prescribed; its velocity is constant at $v^* = 0.066$ in all three sequential movements. The depth of the indentation is set to $d^* = 4$ and kept constant during the scratching phase. The surface of the substrate lies in the xy -plane. The origin of the Cartesian coordinate system is defined as follows: $z^* = 0$ for the initial unpenetrated surface of the substrate and $x^* = 0$ and $y^* = 0$ in the corner of the simulation domain, cf. Fig 1. The size of the substrate block is $\Delta x^* = 37.3$, $\Delta y^* = 274.2$, $\Delta z^* = 139.6$. It consists of 1.5×10^6 atoms.

The rigid cylindrical indenter has a radius of $R_I^* = 8.1$ and consists of 8.2×10^3 atoms. The length of the cylinder corresponds to the width of the substrate and the width of the simulation domain in x -direction. The substrate block is fixed in the simulation domain by constraining the positions of three atom layers next to the box margins at the bottom and in both positive and negative y -direction. The substrate is initialized as a fcc single crystal, which is the equilibrium lattice for the Lennard-Jones potential at the chosen state point.¹¹³ The substrate has an initial density of $\rho_S^* = 1.07$. The substrate surface has a (100) orientation. The scratching direction is in $[0 \bar{1} 1]$. The indenter is fully submersed in the fluid in all lubricated cases. The fluid consists of 9.0×10^5 molecules, with an initial temperature of $T^* = 0.8$ and an initial pressure after the equilibration (see below) of about $p^* = 0.014$. Also, the substrate has an initial temperature of $T^* = 0.8$. Periodic boundary conditions are applied in both x - and y -direction, whereas a soft repulsive wall confines the simulation box at $z^* = 251.3$ at the top. The soft repulsive wall was implemented by a harmonic potential membrane. The time step was $\Delta\tau^* = 0.0008$.

All atoms in the simulation domain were equilibrated for 1×10^6 time steps before the three sequential movements of the indenter are carried out. The initial temperature was imposed to the entire system – except the indenter – during the equilibration. This temperature was also imposed to four atom layers between the substrate and the fixed layer (cf. Fig. 1) during the indentation, the scratching, and the retraction via velocity scaling. This was done to extract dissipated heat from the system which models the heat flux into the bulk body of the substrate.

Definition of Observables

Different observables were computed from the simulation data and used for comparison of the studied dry and lubricated cases. Their definitions are given in the following.

The total tangential force F_t^* and normal force F_n^* on the indenter are evaluated as the sum of all interactions acting on the indenter in y - and z -direction, respectively. The total forces therefore stem from the indenter-substrate (IS) and the indenter-fluid (IF) interactions:

$$F_t^* = \sum_{i=1}^m \left(F_{y,i}^{\text{IS}*} + F_{y,i}^{\text{IF}*} \right) \quad (3)$$

$$F_n^* = \sum_{i=1}^m \left(F_{z,i}^{\text{IS}*} + F_{z,i}^{\text{IF}*} \right), \quad (4)$$

where m is the total number of atoms of the indenter. Also, the indenter-fluid (IF) forces, i.e. only the first terms in Eq. (3) and (4), are computed and compared to investigate the influence of the lubricant. The COF is calculated as

$$\mu = F_t^* / F_n^*, \quad (5)$$

during the scratching.

The energy balance of the system is

$$\Delta U_S^* + \Delta U_F^* = Q_{\text{Th}}^* + W_I^* + \delta E_{\text{err}}^*, \quad (6)$$

where ΔU_S^* and ΔU_F^* are the changes of the total energy (kinetic energy + potential energy) of the substrate and the fluid, respectively. They are averaged in a time interval $\Delta\tau^*$. Q_{Th}^* is the total heat removed from the system by the thermostat. W_I^* is the work done by the indenter on the system. ΔU_S^* , ΔU_F^* , and Q_{Th}^* are simulation results. δE_{err}^* is a remaining numerical error. W_I^* is computed by numerical integration of the respective total force on the indenter

$$W_I^*(\tau^*) = \int_{\text{indentation}} F_n^*(\tau^*) \, dz + \int_{\text{scratching}} F_t^*(\tau^*) \, dy + \int_{\text{retraction}} F_n^*(\tau^*) \, dz, \quad (7)$$

where the forces F_n^* and F_t^* are defined according to Eq. (3) and (4). All energies and forces were computed every 1000 time steps. The main cause for the remaining numerical error δE_{err}^* in the global energy balance in Eq. (6) is the numerical integration in Eq. (7).

The temperature, the density, and the pressure of the fluid are computed locally during the three-stage scratching process. All three properties are computed as per-atom values by averaging the respective property over the atoms within the cut-off radius of each atom. The average aligned velocity from each per-atom collective is subtracted from the total average kinetic energy for the computation of the local temperature by the thermal motion. The fluid region is divided into bins with the size $\Delta y^* = \Delta z^* = 1.34$ and reaching over the entire box width in x -direction, cf. Fig. 2. The fluid properties are computed bin wise, i.e. averaged over all molecules in a bin over 5,000 time steps. The resulting temperature, density, and pressure profiles are computed every 5,000 time steps.

The thermodynamic state point (temperature, density, and pressure) of the fluid is furthermore evaluated around the chip that is formed by the substrate. As the scratching quickly becomes a quasi-stationary process^{9,62} the computation of the state point was only carried out in that stationary phase of the scratching $335 < \tau^* < 625$ (see results). The thermodynamic state point was computed instantaneously every 10,000 time steps. The temperature, density, and pressure of the fluid were computed as a function of the distance R^* from the chip surface as indicated in Fig. 2. The fluid properties were averaged radially around the chip. The instantaneous chip surface was computed using an alpha shape algorithm.¹¹⁴ In this way, profiles showing the decay of the fluid temperature, density, and pressure in the vicinity of the chip surface into the fluid bulk are obtained, i.e. $T^*(R^*)$, $\rho^*(R^*)$, $p^*(R^*)$ where R^* is the distance to the chip surface. Details of the computation of the functions $T^*(R^*)$, $\rho^*(R^*)$, $p^*(R^*)$ are given in the Appendix.

The decay of the temperature, the density, and the pressure of the fluid from the chip surface

into the bulk fluid is modeled here by an exponential function:

$$T_i^* = T_i^{*\text{bulk}} + (T_i^{*\text{wall}} - T_i^{*\text{bulk}}) \cdot \exp(-R^*/\beta^T), \quad (8)$$

$$\rho_i^* = \rho_i^{*\text{bulk}} + (\rho_i^{*\text{wall}} - \rho_i^{*\text{bulk}}) \cdot \exp(-R^*/\beta^\rho), \quad (9)$$

$$p_i^* = p_i^{*\text{bulk}} + (p_i^{*\text{wall}} - p_i^{*\text{bulk}}) \cdot \exp(-R^*/\beta^p). \quad (10)$$

The three parameters β^k , with $k = T^*, \rho^*, p^*$, were fitted to all lubricated simulations simultaneously. Hence, the decay term $\exp(-R^*/\beta^k)$ is assumed to be independent of the solid-fluid interaction energy. The temperature, density, and pressure in the *bulk* fluid and at the *wall* are adopted from each simulation individually. The normalized decay functions ΔT^* , $\Delta \rho^*$, and Δp^* are defined as

$$\Delta T^* = (T_i^* - T_i^{*\text{bulk}})/(T_i^{*\text{wall}} - T_i^{*\text{bulk}}), \quad (11)$$

$$\Delta \rho^* = (\rho_i^* - \rho_i^{*\text{bulk}})/(\rho_i^{*\text{wall}} - \rho_i^{*\text{bulk}}), \quad (12)$$

$$\Delta p^* = (p_i^* - p_i^{*\text{bulk}})/(p_i^{*\text{wall}} - p_i^{*\text{bulk}}), \quad (13)$$

where $i = 1 \dots 18$ stands for the 18 lubricated cases and $T^{*\text{bulk}}, \rho^{*\text{bulk}}, p^{*\text{bulk}}, T^{*\text{wall}}, \rho^{*\text{wall}}, p^{*\text{wall}}$ for the temperature, density, and pressure in the bulk fluid and directly at the solid-fluid interface, respectively.

The *gap* between the indenter and the substrate is defined as indicated by the dark blue shaded area in Fig. 2 as the volume between the indenter and the substrate at $z^* < 0$ and $y^* > y_p^*$ (cf. Fig. 2), i.e. ahead of the indenter in the scratching direction. The number of trapped fluid molecules N_{gap} in this gap is computed from this definition. The contact between the indenter and the substrate can either be dry (no fluid molecules in the gap) or lubricated (fluid molecules in the gap). The substrate and the indenter surface is analyzed with an alpha shape algorithm¹¹⁴ from the simulation trajectories and a surface profile line is calculated parallel to the y, z -plane.

The chip temperature T_{chip}^* is simply defined as the mean temperature of the chip, where the chip constitutes by all substrate atoms whose positions satisfy the conditions $z^* > 0$ and $y^* > y_p^*$

(cf. Fig. 2). The number of fluid molecules in the gap N_{gap} , the chip temperature T_{chip}^* , and the surface profile line are computed every 10,000 time steps.

Results and Discussion

Mechanical Properties

Fig. 3 shows the total forces on the indenter in normal (a) and tangential direction (b) for the dry and all lubricated cases during the entire contact process as well as the resulting coefficient of friction (c) during the scratching. The color scale is related to the energy of the solid-fluid interaction $\tilde{\epsilon}^*$, i.e. the wetting behavior of the fluid.

In the dry case, the total normal and tangential force F_n^* and F_t^* are zero in the first part of the indentation and in the last part of the retraction in which the indenter is not in contact with the substrate. F_n^* and F_t^* fluctuate around zero in these phases in the lubricated cases, which is due to viscous friction of the fluid. *Stephan et al.*⁹ have shown that the amplitude of these fluctuations is related to the energy of the solid-fluid interaction, which is due to the lateral mobility of the fluid molecules on the indenter surface during the movement through the bulk fluid. This lateral mobility of fluid molecules decreases with increasing energy of the solid-fluid interaction, which can also be expressed by the *slip length*,¹¹⁰ as shown in shear flow simulations studies.^{32,111,115,116}

The total normal force on the indenter F_n^* (cf. Fig. 3 a) increases during the indentation, which is due to elastic and plastic deformation of the substrate when the indenter penetrates into the substrate. The normal force on the indenter reaches a maximum at the end of the indentation and then decreases at the beginning of the scratching as the contact area between the indenter and the substrate decreases. F_n^* then reaches a steady state until the end of the scratching process. The total normal force F_n^* on the indenter quickly decreases to zero during the retraction when the indenter moves out of the contact with the substrate. The most evident influence of the fluid and the energy of the solid-fluid interaction is observed at the beginning of the indentation. The fluid acts as a precursor between the indenter and the substrate during the so-called *squeeze out* of fluid particles between the approaching solid bodies.^{48,59,117} Hence, the total normal force starts

increasing in the lubricated cases before both solids actually get into direct contact. This ability of the fluid clearly increases with increasing energy of the solid-fluid interaction. The bump in the normal force at approximately $\tau^* = 50$ in lubricated cases with particularly high energies of the solid-fluid interaction is due to the squeeze out of a second layer of adsorption molecules on the indenter and the substrate surface. The bump in the normal force occurs when this second adsorption layer is squeezed out of the contact zone (see inset of Fig. 3).

It has already been discussed by *Stephan et al.*⁹ that the presence of a lubricant decreases spikes in the normal force during the indentation that are due to the formation of dislocations in the substrate; this is also observed in the present study.

The tangential force F_t^* (cf. Fig. 3 b) in the dry case makes a jump when the indenter comes into contact with the substrate, which is due to the atomistic nature of the contact¹¹⁸ between the indenter and the substrate atoms in y -direction. The fact that the jump in the tangential force in the dry case is in positive y -direction is therefore random and due to the stochastic thermal motion of the particles, which also holds for the lubricated cases. However, the corresponding jump in the lubricated cases is significantly damped due to the presence of fluid atoms acting as springs between the indenter and the substrate. The tangential force F_t^* increases rapidly as the chip starts to form at the beginning of the lateral movement. As for the normal force on the indenter, the tangential force reaches a steady state during which it strongly fluctuates around a mean value of approximately $F_t^* = -47,000$.

At the beginning of the scratching, the coefficient of friction (cf. Fig. 3 c) increases quickly as the lateral movement starts until it reaches approximately a steady state. The steady state is reached at about $\tau^* = 300$. This holds for the dry case as well as the lubricated cases. Evidently, the coefficient of friction in the lubricated cases is lower than in the dry case at the beginning of the scratching. Vice versa, the coefficient of friction shows a tendency to be lower in the dry case than in the lubricated cases in the steady state phase. The reduction of the coefficient of friction in the lubricated cases in the starting phase is a result of an alteration of the normal and the tangential forces likewise, i.e. the normal force is increased and the tangential force decreased by the presence of a fluid. The increase of the coefficient of friction in the lubricated cases during the

steady state phase, on the other hand, is mainly a result of an increased tangential force. This is due to additional viscous friction in the lubricated cases and individually stamped fluid molecules into the substrate surface.^{9,119}

The average forces and coefficient of friction during the two characteristic phases are summarized in Fig. 4 a), b), and c), respectively, as a function of the energy of the solid-fluid interaction with respect to the dry case. Two regimes are distinguished: the lubricated phase ($142 < \tau^* < 335$), during which fluid molecules are present in the gap; and the steady state phase ($335 < \tau^* < 625$), during which the contact zone is essentially dry.

The presence of a lubricant significantly decreases the coefficient of friction (27%) during the starting phase of the scratching. Vice versa, the presence of a lubricant increases the coefficient of friction once the contact zone is essentially dry (15%). The decreased coefficient of friction in the starting phase ($142 < \tau^* < 335$) is a consequence of a combination of an increased normal force and a decreased tangential force compared to the dry case. The increased coefficient of friction in the lubricated cases compared to the dry case during the steady state phase ($335 < \tau^* < 625$) on the other hand is mainly a result of an increased tangential force. The energy of the solid-fluid interaction does interestingly not significantly influence the average forces and coefficient of friction. This is in contrast to the well established strong influence of the solid-fluid interaction on the friction behavior in Couette shear flow systems, cf.^{31–33,110,111,115}

Fig. 5 a) and b) show the resulting normal and tangential forces between the indenter and the fluid. The normal force is highly correlated with the energy of the solid-fluid interaction $\tilde{\epsilon}^*$, while the tangential force shows no systematic dependency on the energy of the solid-fluid interaction. This can be attributed to lubricant molecules that are trapped in the gap between the indenter and the substrate during the indentation phase, before they get squeezed out during the steady state phase of the scratching. The amount of trapped fluid molecules remaining in the gap between both solids increases with increasing energy of the solid-fluid interaction (cf. Fig. 5 c)), which leads to the increasing contribution of the indenter-fluid force to the total force on the indenter in normal direction.

The increase of the normal indenter-fluid force during the indentation is fairly smooth, which

is due to a pressure built-up in the lubrication gap. On the contrary, the decay of the normal indenter-fluid force at the beginning of the scratching ($142 < \tau^* < 300$) shows strong fluctuations. Each spike is due to lubricant molecules being abruptly pushed out of the lubrication gap, which is analog to the classical stick-slip behavior.^{120,121} After the squeeze-out of the fluid out of the contact zone, both the normal and the tangential indenter-fluid force exhibit only small fluctuations. The tangential force fluctuates around approximately $F_t^{*IF} = -100$, the normal force around approximately $F_n^{*IF} = 400$. This is in both cases less than 1% of the corresponding total force (cf. Fig. 3). The increase in the total normal force in the lubricated cases compared to the dry case is attributed to the fluid molecules constantly filling the rear edge behind the indenter in moving direction and pushing the indenter upwards. The contribution of the fluid viscous friction can be estimated from the end of the retraction phase, where the indenter only interacts with the fluid. The average normal force due to the viscous friction is therefore approximately $F_n^{*IF} = 200$.

The tangential fluid-indenter forces F_t^{*IF} show very large fluctuations in the starting phase of the scratching ($142 < \tau^* < 300$), nevertheless a clear tendency of these fluctuations to negative tangential forces can be observed, cf. Fig. 5 b). This trend is a result of the squeeze-out of fluid molecules out of the lubrication gap, while the large fluctuations stem from lubricant molecules being jammed between the indenter and the substrate. Also from Fig. 5 c) it becomes clear that the squeeze-out time is independent from the energy of the solid-fluid interaction $\tilde{\epsilon}^*$.

The reduction of the coefficient of friction in the lubricated cases during the starting phase is attributed to the built lubrication layer in the direct vicinity of the contact zone (cf. Fig. 5 c). The increased coefficient of friction in the lubricated cases during the steady state phase is attributed to viscous friction in the fluid, which is not present in the dry case on the one hand and individual fluid molecules stamped into the substrate surface^{9,119} on the other hand.

Fig. 6 shows the number of trapped fluid molecules in the gap as defined in Fig. 2 at the very end of the indentation ($\tau^* = 142$) as a function of the energy of the solid-fluid interaction $\tilde{\epsilon}^*$. Starting at no coupling between fluid and solid molecules, i.e. $\tilde{\epsilon}^* = 0$, the number of trapped molecules increases with increasing energy of the solid-fluid interaction until it reaches a plateau at approximately $\tilde{\epsilon}^* = 0.75$ where, according to *Becker et al.*,⁶⁸ total wetting is reached in the

investigated Lennard-Jones system. The number of trapped fluid molecules in the gap is therefore strongly correlated with the contact angle that a droplet forms on the substrate.⁶⁸ In the regime of energies of the solid-fluid interaction where total wetting is reached, i.e. $\tilde{\epsilon}^* \geq 0.75$, the amount of trapped fluid molecules does not further increase with increasing energy of the solid-fluid interaction. The intermediator-load of the fluid molecules between the indenter and the substrate during the indentation is limited by the energy of the solid-fluid interaction in the wetting regime of changing contact angle, i.e. $0 < \tilde{\epsilon}^* < 0.75$. Whereas in the regime of total wetting ($\tilde{\epsilon}^* \geq 0.75$), the fluid internal pressure becomes the limiting factor, i.e. the fluid's dispersion energy ϵ_F .

Energy Balance

Fig. 7 shows the work done by the indenter until the end of the indentation as a function of the energy of the solid-fluid interaction $\tilde{\epsilon}^*$. The work done by the indenter in the lubricated cases is given with respect to the work done by the indenter in the dry case. The work done during indentation follows a clear linear trend with increasing energy of the solid-fluid interaction and can be approximated well by

$$W_{\text{I.lub}}^*/W_{\text{I.dry}}^* = a + b \cdot \tilde{\epsilon}^* . \quad (14)$$

The lubricated case with $\tilde{\epsilon}^* = 0$ requires slightly more indentation work than the dry case. The remaining offset compared to the dry case can be attributed to the pure squeeze-out (microflow followed by viscous friction and dissipation) of fluid molecules, as no adsorption bonds have to be broken in the case of $\tilde{\epsilon}^* = 0$. The increasing work done by the indenter with increasing energy of the solid-fluid interaction is mainly due to the decreasing lateral mobility of the fluid molecules on the solid surfaces.^{9,115} This is due to the fact that the adsorption bonds for $\tilde{\epsilon}^* > 0$ between the fluid and both solids (indenter and substrate) have to be broken while both solids approach each other, i.e. stick-slip behavior.^{120,121} The work done by the indenter during the scratching does not show such a clear trend due to strong fluctuations of the tangential forces during the scratching (not shown for clarity). The viscous friction in the fluid has a minor influence on the studied

contact process.

Fig. 8 shows the cumulative energy balance of the entire contact process (cf. Eq. (6)), comparing the dry and the lubricated cases. Since the absolute values of each contribution are mainly due to the kinematics of the process (speed of the indenter, size and shape of the indenter, indentation depth etc.), the relative contribution of the energy partitions are shown and discussed here. All properties of the energy balance W_I^* , ΔU_S^* , ΔU_F^* , and Q_{Th}^* are normalized at each time step during the simulation by the work done by the indenter at the end of the contact process $W_{I,dry}^*(\tau^* = 809)$ in the dry case:

$$\Delta E_{\text{norm}}(\tau^*) = \frac{Z(\tau^*)}{W_{I,dry}^*(\tau^* = 809)} \quad \text{with } Z = W_I^*, \Delta U_S^*, \Delta U_F^*, Q_{Th}^*. \quad (15)$$

This is done for the dry case as well as for all lubricated cases. For clarity, the lubricated cases are combined to the respective color-shaded area. Systematic trends of the energy contributions with varying the energy of the solid-fluid interaction are indicated by arrows. Overall, the energy of the solid-fluid interaction has a minor influence on the energy balance compared to the presence of a fluid in general.

The work done by the indenter corresponds to the energy contribution added to the simulation domain during the contact process. This energy input splits into the heating of the fluid, the heating of the substrate, plastic and elastic deformation of the substrate, and the energy flux into the thermostat layer. The latter describes the heat flux into the bulk material of the substrate.

During the indentation, approximately 81% of the work done by the indenter goes into plastic and elastic deformation of the substrate and its heating up, i.e. the change of the internal energy of the substrate. 6% of the work done by the indenter goes into heating up of the fluid in the lubricated cases and approximately 13% goes into the thermostat layer of the substrate during the indentation.

Throughout the scratching, the internal energy of the substrate fluctuates around an average value, as the average temperature of the substrate quickly reaches a stationary state during the scratching in the applied simulation scenario.⁶² The dissipated energy, which is due to the friction

in the contact zone, therefore goes either into the thermostat layer of the substrate or into the lubricant, if such is present. The thermal energy removed from the simulation box via the thermostat layer in the dry case exceeds the different lubricated cases during the process at most times – especially at the very end of the contact process. Only in the lubricated case with $\tilde{\varepsilon}^* = 0$, more heat is removed via the thermostat (not shown for clarity), as the thermal coupling between the substrate and the fluid is very weak.^{122,123}

The fluid has absorbed between 10 and 15% of the work done by the indenter by the end of the scratching phase depending on the energy of the solid-fluid interaction. The thermostat layer of the substrate has by then removed 85% of the work done by the indenter out of the simulation domain in the dry case. The heat flux into the thermostat layer is significantly reduced in the lubricated cases compared to the dry case. In the lubricated cases, the thermostat layer removed approximately 70% of the work done by the indenter out of the simulation domain. This cooling effect of the lubricant thereby significantly reduces the heat impact into the substrate compared to the dry case. The reason for the reduced heat impact on the substrate’s thermostat layer by the lubricant is twofold; first, the fluid reduces friction during the scratching and thereby reduces dissipation of energy, cf. the work done by the indenter in Fig. 8. Second, the substrate thermostat removes all dissipated energy from the simulation domain in the dry case, whereas in the lubricated cases, also the fluid absorbs a portion of the dissipated energy.

The work done by the indenter monotonously increases during the scratching until the beginning of the retraction. At the beginning of the retraction, the substrate does work on the indenter and the total energy of the substrate decreases, as the substrate can relax from its elastic deformation. The energy contained in the elastic deformation can thereby be estimated to be approximately 7% of the total work done by the indenter during the process.

The substrate thermostat layer removed more energy in the dry case compared to most lubricated cases by the end of the contact process. The thermostat layer keeps removing energy from the simulation domain during the retraction of the indenter, as the initial temperature is imposed to this layer. Since the lubricant itself is not temperature controlled and energy keeps being removed via the thermostat layer of the substrate during the retraction, a total heat flux

from the fluid to the substrate actually slightly cools the fluid during the retraction.

The energy partition observed here might however change when more realistic systems are investigated, e.g. grain boundaries in the substrate instead of a single crystal^{24,82} and a rough surface instead of an atomistically flat one.

The energy of the solid-fluid interaction $\tilde{\epsilon}^*$ has only a minor influence on the energy balance of the process. However, some trends are indicated as arrows in Fig. 8 for clarity. The work done by the indenter during the indentation depends on the energy of the solid-fluid interaction (see also Fig. 6). The increase of the internal energy of the fluid during the scratching slightly increases as the energy of the solid-fluid interaction increases. Multiple superimposing phenomena are the reason for this: the Kapitza resistance at the substrate-fluid interface decreases with an increasing energy of the solid-fluid interaction^{122,124} due to a stronger thermal coupling. This enhances the heat flux from the chip into the fluid with increasing energy of the solid-fluid interaction. Also the energy of the solid-fluid interaction has an influence on the thermodynamic state point of the fluid close to the chip (see below), which accordingly influences the thermal conductivity of the fluid and thereby the heat flux. A further phenomenon that influences the heating up of the fluid is the dependency of the lateral mobility of the fluid molecules on the energy of the solid-fluid interaction.⁹ Hence, an increasing energy of the solid-fluid interaction leads to an increasing dissipation in the adsorbed fluid layer.

The energy of the solid-fluid interaction $\tilde{\epsilon}^*$ of the fluid has a significant influence on the heat input into the bulk substrate, which is modeled by the thermostat layer of the substrate. The heat input into the substrate is reduced by up to 20% for lubricated cases compared to the dry case. The main cause for this reduction is the heating up of the fluid. The reduction of friction due to the presence of a lubricant takes place during the starting phase of the scratching (see the discussed mechanical properties above).

Temperature Field and Thermodynamic Properties of the Lubricant

Fig. 9 shows an exemplary snapshot of the temperature, density and pressure field in the fluid during the simulation towards the end of the scratching ($\tau^* = 554$) in the lubricated simulation

with $\tilde{\epsilon}^* = 1.3$. The temperature field is also shown for the substrate. All three thermodynamic state variables were averaged bin wise during 5,000 time steps. Both the temperature and density profile in the fluid are fairly radial symmetric, which legitimizes the radial averaging as introduced in the section *Definition of Observables*. The temperature field, cf. Fig. 9 – top, reveals that the temperature in the substrate decays much faster than in the fluid. This is due to the fact that the heat conductivity in the substrate is about an order of magnitude higher than in the fluid. The maximum temperature is found in the tip of the chip and the adjacent fluid. The pressure is constant in the fluid, except in the direct vicinity of the solid surfaces, i.e. the adsorbed fluid layer. The temperature field in the fluid causes a change in the density compared to the bulk fluid density.

Fig. 10 – top and bottom – show the temperature and density of the fluid in the surrounding of the chip as a function of the distance to the chip surface R^* and the energy of the solid-fluid interaction $\tilde{\epsilon}^*$. Both the temperature and the density field of the fluid weakly depend on the energy of the solid-fluid interaction. Analog to the number of trapped particles (cf. Fig. 6) – the dependency of the temperature field on $\tilde{\epsilon}^*$ can be distinguished in two regimes: In the range of $0 < \tilde{\epsilon}^* < 0.75$, the temperature of the fluid in direct contact with the chip is significantly lower than in the range of $0.75 < \tilde{\epsilon}^* < 1.7$. As the indenter and the chip carry out a relative motion through the fluid, the adsorbed fluid layers experience a lateral shear flow on the surfaces of the chip and the indenter. This leads to an additional source of energy dissipation, cf.,^{109,125} as discussed above. The decreasing lateral mobility of fluid molecules on the solid surfaces with increasing energy of the solid-fluid interaction leads to an increase of this dissipation and generation of heat at the surface, as for example shown by *Kim et al.*¹²⁵ and reviewed by *Krim*.¹⁰⁹ This can be observed as the fluid temperature directly at the chip surface increases with increasing energy of the solid-fluid interaction of the fluid $\tilde{\epsilon}^*$.

Since the simulation scenario is set up in such a way that the entire fluid experiences an isochoric state change, no vaporization of the fluid takes place. But the local state change of the fluid close to the contact zone is not constrained by this boundary condition.

The decay of the temperature, density and pressure of the fluid from the chip surface into the

bulk fluid are reported in Fig. 11. They are normalized as described in the section *Definition of Observables* by the corresponding chip surface and bulk value. All lubricated cases show the same decay into the bulk, except some small fluctuations. Therefore, all lubricated cases are plotted as a collective shaded area for clarity. The bulk pressure is reached already at distances of approximately 3σ from the chip surface. The fluid temperature and density on the other side converge toward their bulk value at distances of approximately 65σ . The decay of the temperature and the density are almost the same.

The decay of all three state variables can be approximated well with the exponential function as indicated by the solid lines. The temperature and density obey almost perfectly exponential functions, cf. Eq. (11) - (13). The exponential fit function for the pressure profiles agrees within the scattering of the normalized pressure profiles from the different simulations.

Fig. 12 shows the average chip temperature during the scratching process of the lubricated cases with respect to the dry reference case as a function of the energy of the solid-fluid interaction, where the chip is geometrically defined as indicated in Fig. 2. The average chip temperature is slightly decreased compared to the dry case for energies of the solid-fluid interaction $\tilde{\epsilon}^* < 1$ (with two exceptions), but is increased for energies of the solid-fluid interaction $\tilde{\epsilon}^* \geq 1$ (one exception). The reduction of the average chip temperature compared to the dry case for $\tilde{\epsilon}^* < 1$ is a result of the heat flux from the chip into the fluid. With an increasing energy of the solid-fluid interaction the average chip temperature increases due to the decreasing lateral mobility of the fluid on the chip surface, which originates from the friction of the adsorbed fluid layers on the chip, cf.^{9,109,115,125} The continuous breaking of adsorption bonds while the indenter and the chip carry out a relative motion through the fluid results in an increasing dissipation in the adsorbed fluid layer with an increasing energy of the solid-fluid interaction. This leads to an increased average chip temperature for $\tilde{\epsilon}^* \geq 1$ compared to the dry case.

Conclusions

The influence of lubrication on a nanoscopic scratching process in a Lennard-Jones model system was investigated by molecular dynamics simulation. Both mechanical and thermal properties were studied. A special focus was on the influence of the energy of the solid-fluid interaction on the dissipation behavior, the resulting heat fluxes, as well as the overall energy balance. This concept study improves the understanding of nanoscopic machining processes in state of the art production processes.^{83,94}

The presence of a lubricant reduces the coefficient of friction by about 25% compared to a dry case while lubricant molecules remain between the indenter and the substrate. This is a result of an increased normal and slightly decreased tangential force in the starting phase. Once the fluid molecules are squeezed out and the contact is essentially dry with ongoing scratching, the coefficient of friction is increased by the presence of a fluid compared to a dry case by approximately 15%. The change of the coefficient of friction by the presence of a fluid was found to be independent of the energy of the solid-fluid interaction. The number of trapped fluid molecules during the indentation is in general a function of the energy of the solid-fluid interaction and the pressure. The first is found to be dominating for lower energies of the solid-fluid interaction, while the latter is dominating for cases where the energy of the solid-fluid interaction is larger than the dispersion energy of the fluid.

The presence of a fluid has a significant influence on the energy balance of the process. The heat impact on the substrate is reduced up to 20% by the presence of a lubricant compared to a dry simulation. This cooling by the fluid is found to be dependent on the energy of the solid-fluid interaction. Two effects contribute to this cooling: first, the fluid reduces the friction during the starting of the scratching and thereby reduces the amount of dissipated energy in the contact zone. Second, a heat flux from the contact zone to the fluid directly cools the contact zone.

The major part of the work done by the indenter dissipates and is removed from the system via the substrate thermostat. The potential energy of the substrate fluctuates in the stationary phase of the scratching but does not steadily increase with the ongoing formation of the chip. The

energy dissipation dominates the energy balance compared to the energy required for the defect generation and plastic deformation.

The temperature, density, and pressure of the fluid are found to be fairly radial symmetric around the formed chip. The temperature gradient from the chip surface into the bulk fluid is furthermore found to induce a density gradient to maintain local thermodynamic equilibrium as far as possible, whereas the pressure reaches the corresponding bulk value very close to the chip surface. Both temperature and density exhibit the same decay behavior from the chip surface to the bulk fluid. For a future work, it would be interesting to investigate how far from the thermodynamic equilibrium the fluid around the chip is by comparing the computed state point with that of an equation of state for the Lennard-Jones fluid, for example that proposed by *Heier et al.*¹²⁶

The presence of a lubricant is found to be beneficial for both the mechanical and the thermal behavior of the contact process. Overall it is found that the energy of the solid-fluid interaction has a surprisingly minor influence on a nanoscopic scratching process, compared to an important influence in shear flow friction simulations.^{31–33,110,111,115}

The insight gained from the simplified model system from the present work can be extended in future work by increasing the complexity to also study the effect of chain like lubricant molecules, grain boundaries in the substrate block, and a realistic surface roughness on the contact process properties.

Appendix – Radial Averaging around Chip

The computation of the temperature, density, and the pressure of the fluid in the vicinity of the chip as functions $T^*(R^*)$, $\rho^*(R^*)$, $p^*(R^*)$ is described in the following. The radial averaging is carried out with respect to the center of mass of the chip. The chip is defined by all substrate atoms whose positions satisfy the conditions $z^* > 0$ and $y^* > y_P^*$ (cf. Fig. 2). The profiles are then sampled over the angle α with an increment of 2° between $\alpha_{\min}$ and $\alpha_{\max}$. $\alpha_{\min}$ is defined as the angle where the radius R^* tangentially touches the indenter and $\alpha_{\max}$ is defined as the angle

where $R^* = 65$ touches the unpenetrated surface of the substrate ahead of the chip, cf. Fig. 2. Before the actual radial averaging, all individual profiles at different angles α are shifted in a way that the distance R^* has its origin $R^* = 0$ at the surface of the chip to take the not perfectly radial shape of the chip into account. The chip surface was computed with the alpha shape method.

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Table 1: Pairwise interaction energies employed in the present study; all interaction energies are reduced by the interaction energy of the fluid $\varepsilon^* = \varepsilon/\varepsilon_F$.

	substrate (S)	indenter (I)	fluid (F)
substrate (S)	^(a) $\varepsilon_S^* = 52$	^(b) WCA	^(c) $\tilde{\varepsilon}^* = 0, 0.1 \dots 1.6, 1.7$
indenter (I)	-	rigid body	^(c) $\tilde{\varepsilon}^* = 0, 0.1 \dots 1.6, 1.7$
fluid (F)	-	-	^(d) $\varepsilon_F/k_B = 175.06 \text{ K}$
	^(a) Lennard-Jones solid – iron; ⁷⁹		
	^(b) Weeks-Chandler-Anderson potential ¹⁰⁸		
	^(c) 18 cases differing in the solid-fluid interaction energy;		
	^(d) Lennard-Jones fluid – methane. ⁷⁴

Figure 1: Setup of the simulation box for the indentation, scratching, and retraction of the indenter – not true-to-scale. The indenter is either in a vacuum environment (dry case) or fully immersed in fluid (18 different lubricated cases differing in the energy of the interaction between the fluid and the solids (substrate and indenter) $\tilde{\epsilon}^*$).

Figure 2: Schematic (not true-to-scale) for the definition of observables used for the investigation of the nanoscopic contact process. The chip is defined as the substrate material above the unpenetrated substrate surface and ahead of the indenter in scratching direction. The thermodynamic state of the fluid is calculated as a function of the distance from the chip surface and averaged over the angle α (purple shaded area). The radial averaging is carried out with respect to the center of mass of the chip (Details are given in the Appendix). The blue shaded area indicates the lubrication gap presumed for the calculation of the fluid molecules trapped in it. The green rectangle indicates the shape of one of the averaging bins for the computation of the temperature, pressure, and density fields in the simulation box.

Figure 3: Total normal (a) and tangential (b) forces on the indenter during the entire contact process and coefficient of friction (c) during the scratching. The black line indicates the dry reference case. The colors of the other lines are coded by the energy of the solid-fluid interaction $\tilde{\epsilon}^*_s$. The dashed lines indicate the beginning and the end of the scratching phase. The inset in (a) highlights the starting phase of the indentation.

Figure 4: Average mechanical forces and coefficient of friction: a) average normal forces, b) average tangential forces, and c) average coefficient of friction as a function of the energy of the solid-fluid interaction $\tilde{\epsilon}^*$. The average mechanical properties were computed as time averages during the starting phase of the scratching ($142 < \tau^* < 335$) and the steady state of the scratching ($335 < \tau^* < 625$). The results from the dry simulation are taken as reference. The starting phase is indicated by blue symbols, the steady state phase by black symbols. Lines are a guide for the eye.

Figure 5: Normal (a) and tangential (b) forces between the indenter and the fluid during the entire contact process. (c) shows the amount of trapped fluid molecules in the gap (as defined in Fig. 2). The color of the lines is coded by the energy of the solid-fluid interaction $\tilde{\epsilon}^*$. The dashed lines indicate the beginning and the end of the scratching phase from left to right. The inset in (a) highlights the starting phase of the indentation.

Figure 6: Maximum number of fluid particles in the gap (as defined in Fig. 2) as a function of the energy of the solid-fluid interaction $\tilde{\varepsilon}^*$. The maximum number of fluid particles is time averaged between $142 < \tau^* < 200$ to compensate large fluctuations, cf. Fig 5 c). The dashed line is a best fit of an exponential function with $N_0 = 126.5$, $A = -101.7$, and $\tilde{\varepsilon}_0^* = 0.422$.

Figure 7: Average work done by the indenter with respect to the dry case until the end of the indentation ($0 < \tau^* < 142$) as a function of the energy of the solid-fluid interaction $\tilde{\varepsilon}^*$. The dashed line is a best linear fit with $a = 1.046$ and $b = 0.228$.

Figure 8: Energy balance of the entire contact process. The solid lines correspond to the dry case, the shaded areas indicate the maximum and minimum of the lubricated cases at each time step. Black corresponds to the work done by the indenter, gray to the internal energy of the substrate, blue to the internal energy of the fluid, and red to the heat removed from the simulation domain via the thermostat layer of the substrate. The vertical dashed lines indicate the beginning of the scratching and the retraction – from left to right.

Figure 9: Thermodynamic properties of the fluid: (top) temperature, (middle) density, and (bottom) pressure field at the simulation time $\tau^* = 554$ from the lubricated simulation with the energy of the solid-fluid interaction $\tilde{\varepsilon}^* = 1.3$. Each variable is averaged over the box length in x -direction, cf. Fig. 2.

Figure 10: Temperature and density field of the fluid as a function of the distance from the chip surface (cf. Fig. 2) and the energy of the solid-fluid interaction $\tilde{\varepsilon}^*$. (Top) shows the temperature, (bottom) the number density. The properties are averaged during the stationary scratching phase ($335 < \tau^* < 625$) and over the angle α as indicated in Fig. 2 and the Appendix.

Figure 11: Thermodynamic properties of the fluid as a function of the distance from the chip surface: (top) temperature, (middle) density, and (bottom) pressure averaged during the stationary scratching phase ($335 < \tau^* < 625$) and the angle α as indicated in Fig. 2 and the Appendix. The shaded areas indicate the maximum and minimum of the different lubricated cases. The profiles are normalized as defined in Eq. (11) - (13). $R^* = 0$ corresponds to the chip surface and $R^* \rightarrow \infty$ corresponds to the bulk fluid. The exponential decay (black solid lines) is characterized by $\beta^T = 16.96$ for the temperature, $\beta^\rho = 16.43$ for the density, and $\beta^p = 0.59$ for the pressure.

Figure 12: Average chip temperature during the steady state of the scratching ($335 < \tau^* < 625$) with respect to the dry case as a function of the energy of the solid-fluid interaction $\tilde{\epsilon}^*$. The chip geometry was calculated as defined in Fig. 2.

Figure 13: Table of contents graphic/ graphical abstract.