NANOSCIENCE AND NANOTECHNOLOGIES: NANOMACHINING

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Contents

Summary

In nano and micromachining processes the actual material removal can be limited to the surface of the workpiece, i.e. only a few atoms or layers of atoms. At this range, inherent measurement problems and the lack of more detailed experimental data are limiting the possibility for developing analytical and empirical models as more assumptions have to be made. On the basis of atomistic contact models, the dynamics of the local material removal process and its impact on the material structure as well as the surface generation can be studied. First pioneering applications in molecular dynamics (MD) indentation and material removal simulation were published between 1989 and 1991. By starting at the atomic level, the considered microscopic material properties and the underlying constitutive physical equations of state in MD provide, in principle, a sufficiently detailed and consistent description of the micro mechanical and thermal state of the modeled material to allow for the investigation of the local tool tip and workpiece contact dynamics. The description of microscopic material properties considers e.g. microstructure, lattice constants and orientation, chemical elements and the atomic interactions. The more universal material representation in MD allows further to go beyond ideal, single crystalline structures and to consider also poly-crystals, defect structures, pre-machined or otherwise constrained workpiece models and non-smooth surfaces. The development of nanomachining processes is currently in its embryonic stage, but is showing its development in the area of machining electronic materials. This chapter highlights the current advances in nano and micromachining and the development of machine tools capable of controlling atomistic features. The chapter also discusses the use of diamond microtools in this quest and also focuses on the

current advances being made in micromanufacturing such as desktop machine tools and ultra stable machining structures.

1. Nanomachining

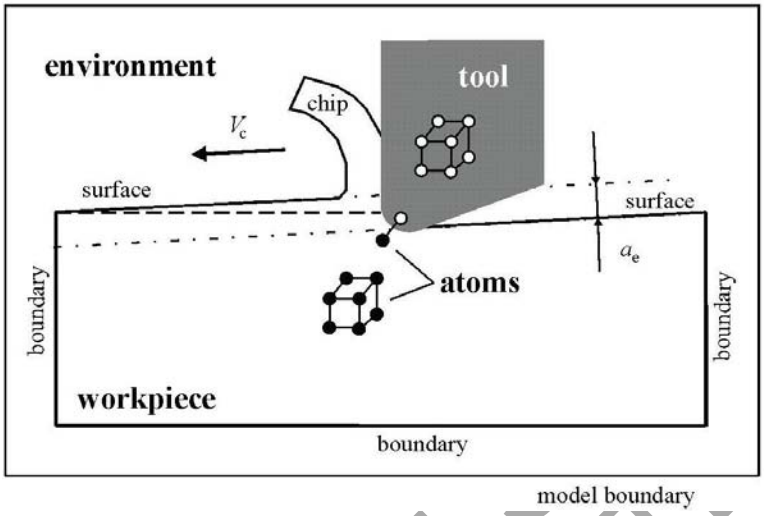

Figure 1. Concept of molecular dynamics simulations

Figure 1 shows a general description of an applied concept for MD cutting process simulation, i.e. the orthogonal cutting condition, and includes the essential elements of MD modeling. Besides the material properties and the interactions between its constituents, the contact and interface conditions, e.g., between tool tip and workpiece as well as with their environment need to be described. Furthermore, the boundary conditions within the model (surfaces vs. bulk material) and the systems boundaries to the surrounding environment are of importance. Table 1 provides a list of the necessary physical elements and principles as well as their area of application in MD modeling. The mathematical description, of the equation of motion in particular, has been included in this listing, since its choice has a major influence on the numerical complexity and the accuracy of calculation. In respect of the application of MD modeling for the nanoscale cutting process simulation, in the following chapter some of the basic elements in Table 1 will be described in more detail first. Then, the design and requirements for state-of-the-art MD cutting process simulations will be discussed and, in the following chapter, the capabilities of MD for the nanoscale material removal process analysis be demonstrated on basis of results of application examples.

Physical element and principle	MD application
Microstructure	Initial configuration
Micro mechanics	Atomic interaction
Dynamics	Equation of motion
Mathematical description	Numerical integration (dynamics)
Thermodynamics	Energy balance of the system
Boundary conditions	Micro mechanical boundaries of the model

Table 1. Area of application of the physical elements and principles in MD modeling

1.1 Basic Elements of Molecular Dynamics Modeling

1.1.1. Material Representation and Microstructure

While the original molecular dynamics theory is well based within the physics, empirical elements were introduced from the material science area in order to match the results of experiments with the theoretical, and so far physical model. The key to computational efficiency of atomic-level simulations lies in the description of the interactions between the atoms at the atomistic instead of the electronic level. This reduces the task of calculating the complex many-body problem of interacting electrons and nuclei like in quantum mechanics to the solution of an energetic relation involving, basically, only atomic coordinates. Accordingly a discrete body or a certain material is described by its chemical elements and by their coordinates. The coordinates provide the information about the atomic arrangement, i.e. the structure of the material, which could be set up, e.g., for a metal on the basis of known lattice structures and lattice constants.

The atomic arrangements in Figure 1 hint on the requirement of a description for all matter involved, primarily for the workpiece and the tool material. Considering the crystal size of typical metals, which range between a few tens to some hundreds of microns in diameter, single crystalline workpiece structures represent reasonable material structures for nanoscale cutting simulations as the tool tip will have to cut over a length of at least 30 000 unit cells before reaching a grain boundary area. However, defects in crystalline structures, like grain boundaries and dislocations, amorphous materials or polymers as well as liquids and gases can also be studied using MD. Although Figure 1 shows a 2D orthogonal cutting set up, the choice of material representation should always be 3D, even if the width of the model is chosen to be only one unit cell wide. The advantage of 2D models lies in the reduced computation time and a somewhat easier visualization of the results. However these advantages are combined with many disadvantages and a great loss of information and meaning of carrying out atomistic simulations. With pure 2D models it is impossible to sufficiently describe the 3D crystalline structure of metals and, hence, no realistic slip system or dislocation motion seems possible and no realistic deformation behavior can be expected. Because of the missing third dimension, 2D simulations result in enhanced, deeper deformation slip as atoms are constrained to accommodate within a plane, in opposite to a 3D model, where each atom has an additional degree of freedom (DoF) to store energy in space.

1.1.2. Atomic Interaction

The central element of the MD code is the calculation of the particle-particle interactions. As it is the most time-consuming part in an MD computer program, it determines the whole structure of the program. Efficient algorithms for the calculation of the interaction are important for systems with a large number of atoms. The interactions between particles are specified by functions that describe the potential energy. Depending on the complexity of a material, and the chosen mathematical description respectively, the potential function may consider many parameters. The goal of the potential function development is, that the functional description and the material

specific set of parameters lead to a self organizing, known structure as a function of the variables of state. This provides the basis as well as the necessary flexibility for carrying out not only phase and structure calculations, but also cutting process calculations at the nanoscale. Potential functions and sets of parameter have to be specified for all possible combinations of interactions, which need to be considered. In the following the principles of the necessary potential functions will be described using the widely applied so-called pair potential functions. The class of the more complex many-body potentials, which is of more importance for the representation of metals, will be discussed only briefly though.

1.1.2.1. Pair Potentials

First van der Waals described a model of a material that can form liquid and solid condensed phases at low temperatures and high pressures. Such condensed phases require both attractive and repulsive forces between atoms. Since the simplest possible representation of many-body interactions is a sum of two-body interactions, the so-called pair potentials were the first potential descriptions of such type. A typical course of the functions is shown in Figure 2.

The best-known pair potential functions are the Lennard-Jones and the Morse potential (see Eq. (1) and Eq. (2)) for which the potential energy ϕ is only a function of the separation or bonding distance $|r|$ between two atoms. The well depth of the functions is given by the parameter ε and D for the minimum potential energy or sublimation energy, while σ and r_0 are constants that define the position of the energy minimum. These parameters are derived from fitting to experimental data like lattice constants, thermodynamic properties, defect energies and elastic moduli. The interaction forces can be derived by calculating the derivative of the potential function, for the pair potential functions only with respect to the separation distance $|r|$.

Lennard-Jones:

$$\phi_{\mathrm{LJ}}(r) = 4\varepsilon\left[(\sigma/r)^{12} - (\sigma/r)^{6}\right] \tag{1}$$

Morse:

$$\phi_{\mathrm{M}}(r) = D\left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}\right] \tag{2}$$

The potentials describe chemically active materials as bonds can be established or cut at the long-range part. They represent reasonable descriptions for two-body forces to the extent, that they account for the repulsion due to overlapping electron clouds at close distance and for attraction at large distances due to dispersion effects. Generally in solids, a shielding effect is expected to make interactions beyond the first few neighbors of limited physical interest. Hence potential functions are commonly truncated at a certain cutoff distance, preferably with a smooth transition to zero (Figure 2), and result

in so-called short-range forces. Besides, the long-ranged Coulomb forces are usually beyond the reach of MD model sizes.

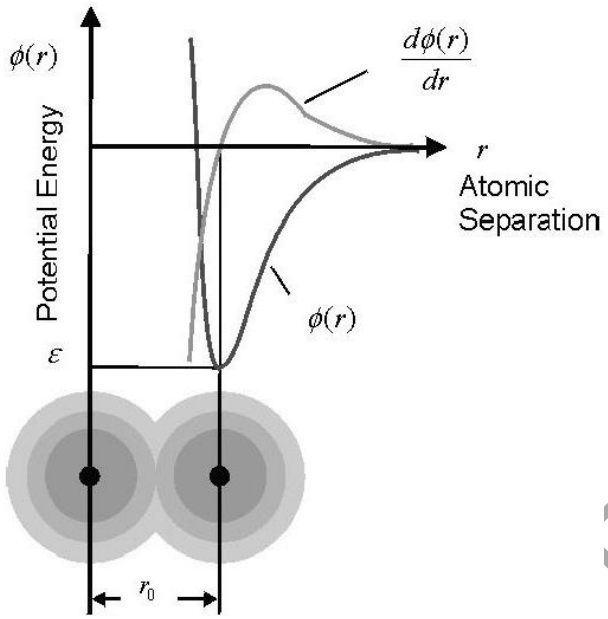

Figure 2. Potential energy as function of atomic separation

1.1.2.2. Many-Body Potentials

The simplicity of the pair potential functions let them appear attractive, for many-atom systems in particular, but they only stabilize structures with equal next neighbor distances, such as fcc and hcp structures, basalt planes and triangular lattices. However, using pair-potentials it is not possible to correctly describe all elastic constants of a crystalline metal. For a better representation of metals many-body interactions need to be included into the function as for example in the well-known potentials following the embedded atom method (EAM). EAM potentials have been developed and tested for complex problems such as fracture, surface reconstruction, impurities and alloying problems in metallic systems.

Also the structure of brittle or non-metallic materials with, for instance, covalent or ionic bonds cannot be satisfactorily described by simple pair-potentials. Ionic materials require special treatment, because Coulomb interactions have poor convergence properties unless the so-called periodic boundaries are implemented with care. For the diamond lattice or the similar cubic zinc blende structure of covalently bonded semi-conductors like silicon and germanium as well as some ceramics, it is necessary to treat the strong directional bonding explicitly by including terms that describe the interaction between three or more atoms considering bond angles and bond order.

1.1.3. Systems Dynamics and Numerical Description

Molecular dynamics comprises macroscopic, irreversible thermodynamics and reversible micro mechanics. The thermodynamic equations form a link between the

micro mechanical state, a set of atoms and molecules, and the macroscopic surroundings, the environment. The thermodynamic equations yield the quantities of system temperature and hydrostatic pressure into the model and allow one to determine energy changes involving heat transfer. In mechanics it is usual to consider energy changes caused by displacement and deformation. By the term "mechanical state" of a microscopic system, a list of present coordinates (r) and velocities (v) of the constituents is meant. For this information about the state of the system to be useful equations of motion, capable of predicting the future, must be available. As the governing equations of motion for a system of constant total energy, Newton's equations of motion can be chosen.

Newton's equations

$$d\left\{v_i\left(t\right)\right\}/dt = 1/m_i * \sum_{i<j}\left\{F_{ij}\left(r_{ij},\alpha,\ldots\right)\right\} \tag{3}$$

of motion:

$$d\left\{r_i\left(t\right)\right\}/dt = v_i\left(t\right) \tag{4}$$

where, $i, j = 1$ to n

The resulting force on an atom i is expressed by an integral over all force contributions F_{ij}. Numerically this is calculated as a sum over all forces acting on each atom i (Eq.(3)). Hence, two bodies at close distance interact through this sum of force contributions in the equation of motion. To advance the atoms in space, the equation of motion has to be integrated with respect to time, once to obtain the new velocity and twice for the new position of each atom. Numerically, this operation is more efficiently carried-out by approximation schemes, for instance using finite difference operators and the so-called Verlet or Stoermer algorithm.

Verlet algorithm:

$$r_i\left(t+\Delta t\right) = r_i\left(t\right) + \Delta t v_i\left(t\right) + 1/\left(2m_i\right)\Delta t^2 F_i\left(t\right) \tag{5}$$

$$v_i\left(t+\Delta t\right) = v_i\left(t\right) + \Delta t/\left(2m_i\right)\left\{F_i\left(t+\Delta t\right) + F_i\left(t\right)\right\}\} \tag{6}$$

where, $i = 1$ to n.

With the present positions ($r_i\left(t\right)$), velocities ($v_i\left(t\right)$) and forces ($F_i\left(t\right)$), first the new positions and forces at time $t+\Delta t$ can be calculated and then the new velocity as well. Given the equations of motion, forces and boundary conditions, i.e. knowing the current mechanical state, it is possible to simulate future behavior of a system. Mathematically this represents an initial value problem. A reasonable distribution of the initial velocities can be obtained from the Maxwell-Boltzmann distribution function.

The dynamic development of the atomic system as a whole determines the instantaneous kinetic state of the system. By relating the average kinetic energy of the atoms (with average velocity v), i.e., their micro mechanical state, to the thermal energy of the system, which is the thermodynamic state, the gas kinetic definition of the system temperature is adopted. From Eq. (7)) the temperature T of a 3D system of atoms can directly be observed or, for a given reference temperature, the kinetic energy in the system be controlled.

$$E_{\text{kin}} = 1/2\, m 1/n \sum v_i^2 = 3/2 * k_{\text{B}} * T = E_{\text{therm}}. \qquad (7)$$

where, $i = 1$ to n

Since the initial choice of the atom configuration is more or less idealistic, i.e. artificial, it does not fit to the Maxwell-Boltzmann distribution from the energetic point of view. The whole system needs to pass through an initial equilibration phase, during which the atom configuration adjusts to the invariants of the system, e.g., total system energy, volume, pressure and/or temperature, and thereby also to the boundary conditions.

1.1.4. Boundary Conditions

Boundaries are an intrinsic, vital part of models. Thermodynamic properties are thought of as characterizing "bulk" matter, which represents enough material so that surface effects and fluctuations can be ignored. To decrease the influences of boundaries, the system size needs to be chosen so that it can be computed. However, the fulfillment of this weak requirement is generally limited by the available CPU power and time. Besides, the option of free surfaces, which would result in a particle cluster in free space if applied to all axes of a Cartesian coordinate system, basically 2 types of boundaries are common in MD simulations: fixed and periodic boundaries. The simplest type, in terms of realization, is the fixed atom boundary which confines all freely propagating atoms inside a closed box of not moving atoms or provides support for them at one or more sides. It is simply realized by taking away the dynamics of such boundary atoms, but keeping the interactions with the freely moving atoms. The consequences of such infinitely hard boundaries for the simulation can be significant as no energy can be passed through the boundary and phonons will be reflected at it. The sole use of hard boundaries represents a poor representation of the surrounding environment / material. Some of the negative effects of hard boundaries can be corrected by placing thermally controlled atom layers between freely moving atoms and a hard boundary.

Periodic boundary conditions (PBC) were introduced to avoid the hard boundary reflection and allow the study of bulk and bulk/interface structures without the strong boundary influence in small models. It is imagined, that the bulk of the material is made of many similar systems along the axis perpendicular to the periodic boundary plane, i.e. there are no surfaces along this axis. The system reacts as if there are identical systems at both sides of the PBC, exposed to the same conditions and changes (see Figure 3). Practically the system is connected to itself and atoms at one side interact with atoms on the other side and form a continuous structure. If deformation in the system requires atoms to slip across the PBC, it transfers from one to the other side of the model. Figure 3 shows a sketch of an indentation model (triangular indenter on a top

of a workpiece), where a one-axis PBC is considered perpendicular to the horizontal axis.

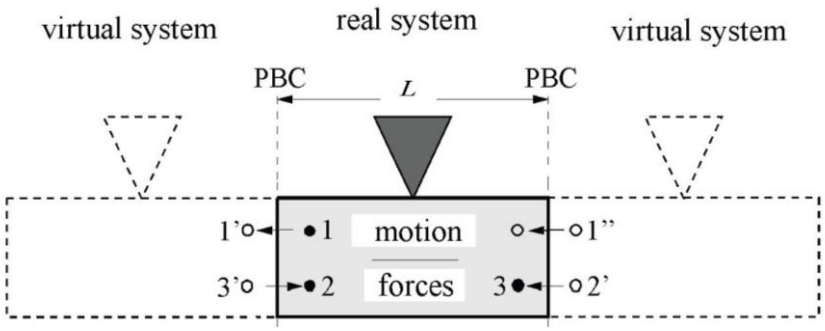

Figure 3. Motion through (atom 1) and forces at (atoms 2-3) a periodic boundary (PBC)

A consequence of periodic boundaries is that energy and phonons are not reflected, but travel through the system by means of the PBC's. One or two-axis PBC can be employed where symmetry axes are available and the lattice structure allows an undisturbed bonding through the PBC planes. Additionally, a deformation compatibility across a PBC has to be fulfilled by an appropriate alignment of preferred slip systems relative to the PBC's, in order to avoid artificial deformation patterns.

The following results were all obtained by using 3D MD models, EAM potential functions and PBC's in one or two axes, even if the width of the underlying MD model was only a few lattice constants wide, following the approach of the orthogonal cutting process condition.

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Biographical Sketch

Professor Mark J. Jackson is an Associate Professor of Mechanical Engineering and University Faculty Scholar at Purdue University, Faculty Associate at Y12 National Security Complex at Oak Ridge, Tennessee, Faculty Associates at the Birck Nanotechnology Centre and Centre for Advanced Manufacturing at Purdue University, and Visiting Professor at Harbin Institute of Technology, China. Born in Widnes, Lancashire, England, in 1967, Doctor Jackson began his engineering career in 1983 when he studied for his O.N.C. part I examinations and his first-year apprenticeship-training course in mechanical engineering. After gaining his Ordinary National Diploma in Engineering with distinctions and I.C.I. prize for achievement, he read for a degree in mechanical and manufacturing engineering at Liverpool Polytechnic and spent periods in industry working for I.C.I. Pharmaceuticals, Unilever Industries, and Anglo Blackwells. After graduating with a Master of Engineering (M. Eng.) degree with

Distinction under the supervision of Professor Jack Schofield, M.B.E., Doctor Jackson subsequently read for a Doctor of Philosophy (Ph. D.) degree at Liverpool in the field of materials engineering focusing primarily on microstructure-property relationships in vitreous-bonded abrasive materials under the supervision of Professor Benjamin Mills. He was subsequently employed by Unicorn Abrasives' Central Research & Development Laboratory (Saint-Gobain Abrasives' Group) as materials technologist, then technical manager, responsible for product and new business development in Europe, and university liaison projects concerned with abrasive process development. Doctor Jackson then became a research fellow at the Cavendish Laboratory, University of Cambridge, working with Professor John Field, O.B.E., F.R.S., on impact fracture and friction of diamond before becoming a lecturer in engineering at the University of Liverpool in 1998. At Liverpool, Dr. Jackson established research in the field of micro machining using mechanical tools, laser beams, and abrasive particles. At Liverpool, he attracted a number of research grants concerned with developing innovative manufacturing processes for which he was jointly awarded an Innovative Manufacturing Technology Centre from the Engineering and Physical Sciences Research Council in November 2001. In 2002, he became associate professor of mechanical engineering and faculty associate in the Centre for Manufacturing Research, Centre for Electric Power, and Centre for Water Resources and Utilization at Tennessee Technological University (an associated university of Oak Ridge National Laboratory), and a faculty associate at Oak Ridge National Laboratory. Dr. Jackson was the academic adviser to the Formula SAE Team at Tennessee Technological University. At Tennessee Technological University, Dr. Jackson established the NSF Geometric Design and Manufacturing Integration Laboratory. In 2004 he moved to Purdue University as Associate Professor of Advanced Manufacturing in the Department of Mechanical Engineering Technology, Birck Nanotechnology Centre, and the Centre for Advanced Manufacturing. In 2005, Dr. Jackson established the Advanced Manufacturing Technology Laboratory at Purdue University. In the Fall of 2005, Dr. Jackson was jointly awarded a U. S. Army Research Office award to establish the Advanced Manufacturing Laboratory at Purdue Discovery Park. Dr. Jackson is also working with Purdue's Krannert Business School on aspects of commercialising micro and nanotechnologies. Dr. Jackson is Director of the Advanced Manufacturing Laboratory in the College of Technology. Doctor Jackson is active in research work concerned with understanding the properties of materials in the field of micro scale metal cutting, micro and nano abrasive machining, and laser micro machining. He is also involved in developing next generation manufacturing processes and biomedical engineering. Doctor Jackson has directed, co-directed, and managed research grants funded by the Engineering and Physical Sciences Research Council, The Royal Society of London, The Royal Academy of Engineering (London), European Union, Ministry of Defence (London), Atomic Weapons Research Establishment, National Science Foundation, N.A.S.A., U. S. Department of Energy (through Oak Ridge National Laboratory), Y12 National Security Complex at Oak Ridge, Tennessee, and Industrial Companies, which has generated research income in excess of £18 million ($25 million). Doctor Jackson is Director of Research and Vice President of Micro Machinists, LLC., which is established to develop next generation nano and micro machine tools and cutting tools for nanotechnology applications.