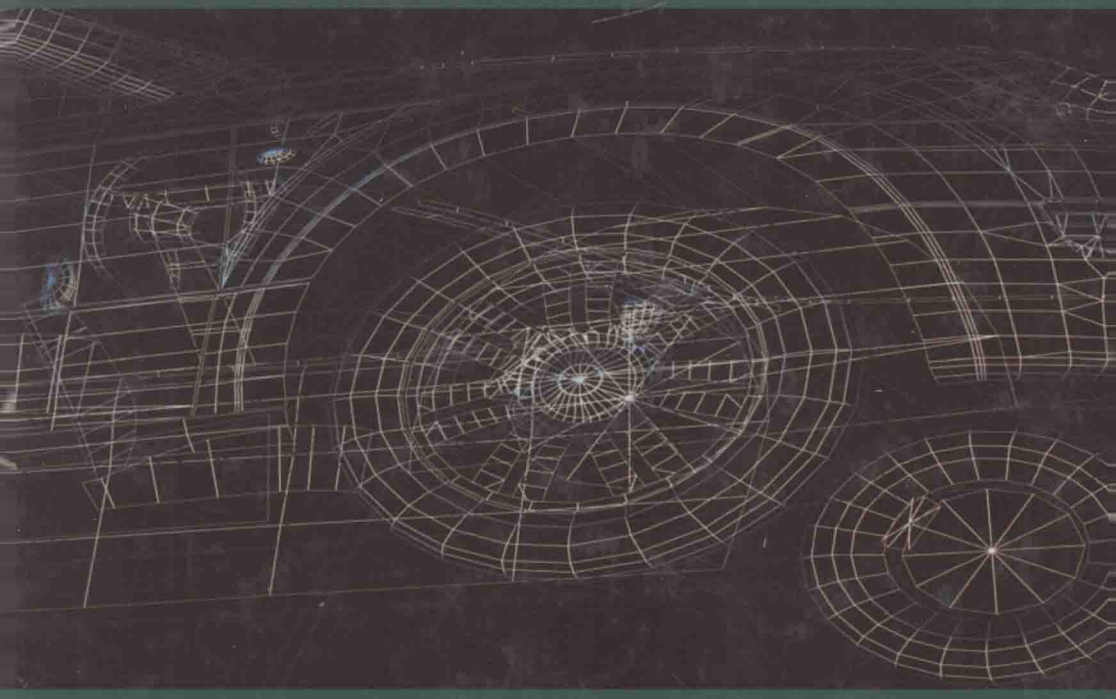
Nano and Micromachining

Edited by
J. Paulo Davim and Mark J. Jackson



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Nano and Micromachining

Preface

At this moment in time, it is difficult to obtain an exact definition of nano and micromachining. Nanomachining is a recent nanotechnology that involves changing the structure of nano-scale materials or molecules. The Institute of Nanotechnology (UK) defines nanotechnology as "science and technology where dimensions and tolerances in the range of 0.1 nanometer (nm) to 100 nm play a critical role". Micromachining (performing various cutting processes or grinding operations on workpiece in micro-scale) covers techniques used, for example, in manufacturing the miniaturized devices and moving parts into which microelectronic circuitry is integrated. Unlike micromachining, where portions of the structure are removed or modified, nanomachining involves only changing the structure of nanoscale materials or molecules.

This book aims to provide the fundamentals and the recent advances in nano and micromachining for modern manufacturing and engineering.

Chapter 1 provides the fundamentals of molecular dynamics for nanoscale cutting. Chapter 2 contains information on ductile mode cutting of brittle materials and generic descriptions of the significant aspects involved – mechanism, chip formation and machined surfaces. Chapter 3 covers diamond tools used in micromachining. Chapters 4 and 5 contain information on convention machining processes, microturning, microdrilling, micromilling, microgrinding and ultra-precision processes. Chapter 6 focuses on a non-conventional process – laser micromachining. Chapter 7 covers the evaluation of subsurface damage in nano and micromachining. Finally, Chapter 8 is dedicated to applications of nano and micromachining in industry.

The present book can be used as a textbook for a final year undergraduate engineering course or specifically for nano and micromanufacturing (machining) at postgraduate level. Also, this book can serve as a useful reference for academics,

manufacturing and materials researchers, manufacturing and mechanical engineers, as well as professionals in nano and micromanufacturing and related industries. The scientific interest of this book is evident for many important research centers, laboratories and universities in the world. Therefore, it is hoped that this book will encourage and enthuse other research in this recent field of science and technology.

The editors acknowledge their gratitude to ISTE-Wiley for this opportunity and for their professional support. Finally, we would like to thank all the chapter authors for their availability for this work.

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October 2008

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Table of Contents

Chapter 1

Nanoscale Cutting

1.1. Introduction

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 limit 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.

The first pioneering applications in molecular dynamics (MD) indentation and material removal simulation were published between 1989 and 1991 [BEL 91, IKA 91, HOO 90, LAN 89]. 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 micromechanical and thermal state of the modeled material to allow for the investigation of the local tool tip/workpiece contact dynamics [HOO 91, RAP 95]. The description of microscopic material properties considers, e.g., the microstructure, lattice constants and orientation, chemical elements and the atomic interactions.

Chapter written by Rüdiger RENTSCH.

The more universal material representation in MD further allows us to go beyond ideal, single crystalline structures and to also consider polycrystals, defect structures, pre-machined or otherwise constrained workpiece models and non-smooth surfaces [DAW 84, REN 95-1, REN 95-3, YIP 89]. Various application-specific boundary conditions may be applied [HOO 91, RAP 95, YIP 89]. In recent years the number of applications considering quantum mechanics for the interactions between atoms has been steadily increasing. However, here only the more classical atomistic approach will be presented.

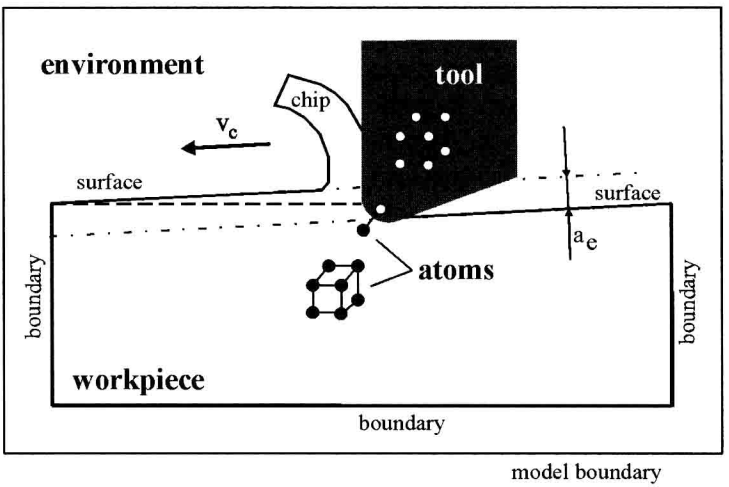

Figure 1.1. *Concept of a molecular dynamics cutting model setup*

Figure 1.1 shows a general description of an often applied concept for MD cutting process simulation, i.e. the orthogonal cutting condition, and includes the essential elements of MD modeling. In addition to 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 system boundaries to the non-modeled environment are of importance. Table 1.1 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 1.1 will be described in more detail first. Then, in section 1.3, the design and requirements for state-of-the-art MD cutting process simulations will be discussed and, in the following section, the capabilities of MD for the nanoscale material removal process analysis will be demonstrated on the basis of results of application examples. Some aspects regarding significant advances and recent developments in MD material removal process simulation will be discussed in section 1.5, before the summary and outlook of this contribution is given.

Physical element/ principle	**Application in MD**
• microstructure	initial configuration
• micro-mechanics	atomic interaction
• dynamics	equation of motion
• mathematical description	numerical integration (dynamics)
• thermodynamics	energy balance of the system
• boundary conditions	micromechanical boundaries of the model

Table 1.1. *Application area of the physical elements and principles in MD modeling*

1.2. Basic elements of molecular dynamics modeling

1.2.1. *Material representation and microstructure*

While the original molecular dynamics theory is well based within physics, empirical elements were introduced from the materials science field 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 as in quantum mechanics to the solution of an energetic relation involving, basically, only atomic coordinates [HOO 91]. 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 1.1 hint at 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 several hundred 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 [DAW 84, REN 95-3, REN 06, SHI 94, YIP 89], amorphous materials [GLO 95, RAP 95] or polymers as well as liquids and gases [ALL 87, RAP 95] can also be studied using MD. Although Figure 1.1 shows a 2D orthogonal cutting setup, 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 calculation 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 opposition to a 3D model, where each atom has an additional degree of freedom (DoF) to store energy in space [REN 01].

1.2.2. *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 (see [ALL 87, RAP 95]).

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 state variables. 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 parameters have to be specified for all possible combinations of interactions that 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 however be discussed only briefly.

1.2.2.1. *Pair potentials*

First, van der Waals described a model of a material which can form liquid and solid condensed phases at low temperatures and high pressures. Such condensed phases require both attractive and repulsive forces between atoms [HOO 91]. 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 this type. A typical course of the functions is shown in Figure 1.2.

The best known pair potential functions are the Lennard-Jones and the Morse potentials (see equation [1.1] and equation [1.2]) 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 are given by parameters ε and D for the minimum potential energy or sublimation energy, while σ and r_o 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: $$\Phi_{LJ}(r) = 4 * \varepsilon * [(\sigma / r)^{12} - (\sigma / r)^{6}] \quad [1.1]$$

Morse: $$\Phi_{M}(r) = D * [e^{-2\alpha(r-ro)} - 2e^{-\alpha(r-ro)}] \quad [1.2]$$

The potentials describe chemically active materials as bonds that 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. Thus, potential functions are commonly truncated at a certain cutoff distance, preferably with a smooth transition to zero (see Figure 1.2), and result in so-called short-range forces. In addition, the long-range Coulomb forces are usually beyond the reach of MD model sizes [HOO 91].

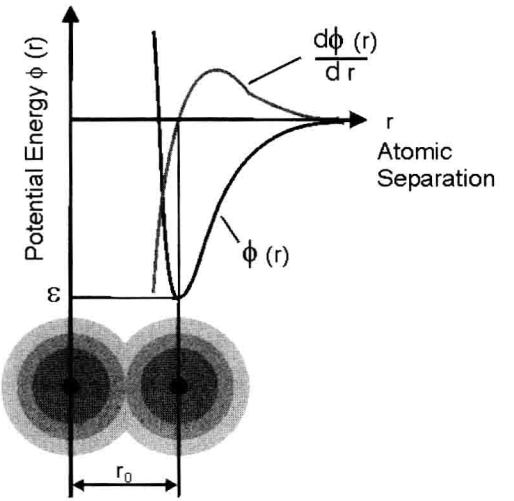

Figure 1.2. *Potential energy according to atomic separation*

1.2.2.2. *Many-body potentials*

The simplicity of the pair potential functions make them appear attractive, for many-atom systems in particular, but they only stabilize structures with equal next neighbor distances, like 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) [DAW 84, FIN 84]. In all of the following MD results, the Finnis-Sinclair-type EAM potential by Ackland *et al.* was employed for the workpiece-workpiece interactions [ACK 87]. EAM potentials have been developed and tested for complex problems such as fracture, surface reconstruction, impurities and alloying problems in metallic systems.

The structure of brittle or non-metallic materials with, for instance, covalent or ionic bonds can also not 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 (see [ALL 87]). For the diamond lattice or the similar cubic zinc blend 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 (see [TER 90, YIP 89]).

1.2.3. *System dynamics and numerical description*

Molecular dynamics comprises macroscopic, irreversible thermodynamics and reversible micro-mechanics. The thermodynamic equations form a link between the micromechanical state, a set of atoms and molecules, and the macroscopic surroundings, the environment. The thermodynamic equations yield the quantities, system temperature and hydrostatic pressure of the model and allow us 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 we mean a list of present coordinates (r) and velocities (v) of the constituents [HOO 91]. 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, the well-known Newton's equations of motion can be chosen:

$$\text{Newton's equations of motion } d\{v_i(t)\} / dt = 1 / m_i * \Sigma_{i<j}\{F_{ij}(r_{ij},\alpha,...)\} \qquad [1.3]$$

$$d\{r_i(t)\} / dt = v_i(t) \qquad [1.4]$$

with 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 (equation [1.3]). 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 [ALL 87, HOO 91]:

$$\text{Verlet algorithm: } r_i(t+\Delta t) = r_i(t) + \Delta t * v_i(t) + 1/(2*m_i) * \Delta t^2 * F_i(t) \qquad [1.5]$$

$$v_i(t+\Delta t) = v_i(t) + \Delta t /(2*m_i) * \{F_i(t+\Delta t) + F_i(t)\} \qquad [1.6]$$

with i = 1 to n.

With the present positions ($r_i(t)$), velocities ($v_i(t)$) and forces ($F_i(t)$), first the new positions and forces at time $t+\Delta t$ and then the new velocity can be calculated. Given the equations of motion, forces and boundary conditions, i.e. knowing the current mechanical state, it is possible to simulate the 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.