Surface Engineered Surgical Tools and Medical Devices

Surface Engineered Surgical Tools and Medical Devices

Edited by

Mark J. Jackson
Purdue University
West Lafayette, IN, USA

Waqar Ahmed
University of Ulster
Newtownabbey, UK

Springer

Mark J. Jackson
Purdue University
Birck Nanotechnology Center
College of Technology
West Lafayette, IN, USA

Waqar Ahmed
University of Ulster
NIBEC
Newtownabbey, UK

Library of Congress Control Number: 2007920041

ISBN 978-0-387-27026-5 e-ISBN 978-0-387-27028-9

Printed on acid-free paper.

9 8 7 6 5 4 3 2 1

springer.com

Foreword by Sir Harold W. Kroto

The new millennium has seen the birth of a new perspective that conflates research in solid-state physics, biological science as well as materials engineering. The perspective is one that recognizes that future new advances in all these areas will be based on a fundamental understanding of the atomic and molecular infrastructure of materials that has resulted from two centuries of chemistry. Major advances will be achieved when the novel behavior, in particular the quantum mechanical behavior, that nanoscale structures possess, can be controlled and harnessed.

To go with this new perspective the conflated fields have acquired a new name - Nanoscience and Nanotechnology (N&N). The promise of developing functional devices at the molecular and atomic scale is now becoming a reality. However, a massive effort is still needed in order to control the fabrication of such novel nanodevices and nanomachines and exploit processes based on quantum mechanical laws. The next decade should see the emergence of new technologies based on nano-systems with not only improved but hopefully also fundamentally new physico-chemical properties produced at reasonable costs. Experimental and theoretical research should lead to industrial applications yielding important breakthroughs. If universities, independent research centers, government agencies and innovative industrial organizations invest time and resources imaginatively in this multidisciplinary adventure, a highly synergistic process will ensue in the development of these new technologies.

Nanotechnology is the ability to manipulate atoms and molecules to produce nanostructured materials and functional nanocoatings on biomedical devices and surgical tools. Nanotechnology is likely to have a significant effect on the global economy and on society in this century, and it promises to make breakthroughs in the biological and medical sciences.

This book contains chapters that focus not only on fundamental advances that are taking place but also on important applications, in particular in the biomedical field that promise to revolutionize a wide range of technologies in the 21^{st} century. The unique properties that emanate from nanoscale structures are immensely varied and in the next decade nanoscience and nanotechnology will give birth to a vast new range of exciting technological applications that promise to help the creation of a sustainable socio-economic environment.

Professor Sir Harold W. Kroto, FRS
Nobel Laureate, Chemistry 1996

Preface

Medical devices and surgical tools that contain micro and nanoscale features allow surgeons to perform clinical procedures with greater precision and safety in addition to monitoring physiological and biomechanical parameters more accurately. While surgeons have started to master the use of nanostructured surgical tools in the operating room, the impact and interaction of nanomaterials and nanostructured coatings has yet to be addressed in a comprehensive manner.

Nobel Laureate Richard Feynman's revolutionary vision on nanotechnology was captured in a paper published in the February 1960 issue of Caltech's journal, '*Engineering and Science*'. In this paper, Feynman speaks about manipulating atoms and constructing products atom-by-atom, and molecule-by-molecule. Feynman describes the scaling down of lathes and drilling machines, and talks about drilling holes, turning, molding, and stamping parts. Even in 1959, Feynman describes the need for micro and nanofabrication as the basis for creating a microscopic world that would benefit mankind. Nanotechnology encompasses technology performed at the nanoscale that has real world applications. Nanotechnology will have a profound effect on our society that will lead to breakthrough discoveries in materials and manufacturing, medicine, healthcare, the environment, sustainability, energy, biotechnology, and information technology.

President Bill Clinton talked about the exciting promise of nanotechnology in January 2000, and later announced an ambitious national nanotechnology initiative (NNI) that was enacted in 2001 with a budget of $497 million to promote nanoscale research that would benefit society. The purpose of this book is to present information and knowledge on the emerging field of surface engineered biomedical devices and surgical tools. The book is written in the spirit of scientific endeavor outlined by Richard Feynman, who stated that one of the greatest challenges to scientists in the field of miniaturization is the manufacture of objects for medical applications using techniques such as turning, molding, stamping, and drilling. The book presents information on surface engineered surgical tools and medical devices that looks at the interaction between nanotechnology, nanomaterials, and tools for surgical applications. Chapters of the book describe developments in coatings for heart valves, stents, hip and knee joints, cardiovascular devices, orthodontic applications, and regenerative materials such as bone substitutes. Chapters are also dedicated to the performance of surgical tools and dental tools and also describe how nanostructured surfaces can be created for the purposes of improving cell adhesion between medical device and the human body.

The structure of the book is based on matter provided by many colleagues and the author wishes to thank the contributors of this book for helping construct a source of knowledge and information on surface engineered medical devices and surgical tools and for granting the editors permission to use such matter.

Mark J. Jackson
Purdue University

Waqar Ahmed
University of Ulster

October 2006

Contents

List of Authors

Wunmi Ademosu
Thin Film Research Center,
School of Engineering and Science,
University of Paisley,
Paisley, PA1 2BE, Scotland, U.K.
E-mail: *wunmi.ademosu@paisley.ac.uk*

Waqar Ahmed
University of Ulster,
NIBEC,
Newtownabbey, BT 37 0QB,
United Kingdom.
E-mail: *w.ahmed@ulster.ac.uk*

Nasar Ali
University of Aveiro,
Department of Mechanical Engineering,
3810-193 Aveiro, Portugal.
E-mail: *n.ali@mec.ua.pt*

Matej Balazic
Machining Laboratory,
Department of Machining Technology Management,
Faculty of Mechanical Engineering,
University of Ljubljana,
Askerceva 6, SI-1000 Ljubljana,
Slovenia.

D. Bombac
Ul. Metoda Mikuza 12,
SI-1000 Ljubljana, Slovenia.

M. Brojan
Laboratory for Nonlinear Mechanics,
Department of Mechanics,
Faculty of Mechanical Engineering,

University of Ljubljana,
Askerceva 6, SI-1000 Ljubljana,
Slovenia.

J. Anthony Byrne
University of Ulster, NIBEC,
Newtownabbey, BT 37 0QB,
United Kingdom.
E-mail: *j.a.byrne@ulster.ac.uk*

Gil Cabral
University of Aveiro,
Department of Mechanical Engineering,
3810-193 Aveiro, Portugal.

R. Caram Jr.
Department of Materials Engineering,
State University of Campinas,
UNICAMP C.P. 6122, 13083-970 Campinas SP,
Brazil.

M. H. Fernandes
FMDUP – Faculdade de Medicina Dentária da Universidade do Porto, Rua, Dr., Manuel Pereira da Silva,
4200-393 Porto, Portugal.

Juan Gracio
University of Aveiro,
Department of Mechanical Engineering,
3810-193 Aveiro, Portugal.
E-mail: *jgracio@mec.ua.pt*

Rodney G. Handy
Purdue University,
College of Technology,
401 North Grant Street,
West Lafayette, IN 47907-2021, USA.
E-mail: *rhandy@purdue.edu*

N. Sooraj Hussain
INEB - Instituto de Engenharia Biomédica,
Laboratório de Biomateriais, Rua Campo Alegre,
823, 4150 -180, Porto, Portugal.

Mark J. Jackson
Purdue University,
Birck Nanotechnology Center,
College of Technology,
401 North Grant Street,
West Lafayette, IN 47907-2021, USA.
E-mail: *jacksomj@purdue.edu*

Januz Kopac
Machining Laboratory,
Department of Machining Technology Management,
Faculty of Mechanical Engineering,
University of Ljubljana,
Askerceva 6, SI-1000 Ljubljana,
Slovenia.

F. Kosel
Laboratory for Nonlinear Mechanics,
Department of Mechanics,
Faculty of Mechanical Engineering,
University of Ljubljana,
Askerceva 6, SI-1000 Ljubljana,
Slovenia.

Yasmeen Kousar
University of Aveiro,
Department of Mechanical Engineering,
3810-193 Aveiro, Portugal.
E-mail: *y.kousar@mec.ua.pt*

Michael D. Lafreniere
Ohio University,
Chillicothe,
Ohio, USA.
E-mail:

J. C. Madaleno
University of Aveiro,
Department of Mechanical Engineering,
3810-193 Aveiro, Portugal.

Chris Maryan
Manchester Metropolitan University,
Chester Street,

Manchester, M1 5GD, U.K.
E-mail: *c.maryan@mmu.ac.uk*

A. C. Maurício
FEUP – Faculdade de Engenharia da Universidade do Porto,
DEMM, Rua Dr., Roberto Frias, 4200 - 465 Porto, Portugal.

Andrew McLean
School of Engineering and Science,
University of Paisley,
Paisley, PA1 2BE, Scotland, U.K.
E-mail: *andrew.mclean@paisley.ac.uk*

Abraham A. Ogwu
School of Engineering and Science,
University of Paisley,
Paisley, PA1 2BE, Scotland, U.K.
E-mail: *ogwu-ph0@paisley.ac.uk*

Thomas Okpalugo
University of Ulster,
NIBEC,
Newtownabbey, BT 37 0QB,
United Kingdom.
E-mail: *tit.okpalugo@ulster.ac.uk*

Frank Placido
Thin Film Research Center,
School of Engineering and Science,
University of Paisley,
Paisley, PA1 2BE, Scotland, U.K.
E-mail: *frank.placido@paisley.ac.uk*

J. D. Santos
FEUP,
Faculdade de Engenharia da Universidade do Porto,
DEMM, Rua Dr.,
Roberto Frias,
4200 - 465 Porto, Portugal.

Patrick Senarith
Medtronic, Inc,
7000 Central Ave.
Minneapolis, MN 55432
E-mail: *Patrick.Senarith@medtronic.com*

T. Shokuhfar
University of Aveiro,
Department of Mechanical Engineering,
3810-193 Aveiro, Portugal.

A. C. M. Sousa
University of Aveiro,
Department of Mechanical Engineering,
3810-193 Aveiro, Portugal.

Elby Titus
University of Aveiro,
Department of Mechanical Engineering,
3810-193 Aveiro, Portugal.

Thomas J. Webster
Division of Engineering,
Brown University,
Providence, RI USA 02912.
E-mail: *Thomas_Webster@Brown.edu*

Michael D. Whitt
Purdue University,
Mechanical Engineering Technology,
Knoy Hall of Technology, Room 184,
West Lafayette, IN 47907-2021.
E-mail: *mwhitt@purdue.edu*

Chang Yao
Division of Engineering,
Brown University,
Providence, RI USA 02912.
E-mail: *Chang_Yao@Brown.edu*

Nomenclature

AIDS = Acquired Immune Deficiency Syndrome
AFI = Average Fluorescence Intensity
ALP = Alkaline Phosphatase Activity
a-C:H = Hydrogenated amorphous carbon
a-C:H:N = Nitrogen doped hydrogenated amorphous carbon
a-C:H:Si = Silicon doped hydrogenated amorphous carbon
AFM = Atomic Force Microscopy
BMA = Bone Marrow Aspirate
BMP = Bone Morphogenetic Protein
BMU = Basic Multicellular Unit
BSA = Bovine Serum Albumine
BSP = Bone Sialoprotein
CAM = Cell Adhesion Molecule
CCD = Charged Coupled Device
COL I = Collagen type 1
CPD = Contact Potential Difference
PECVD = Plasma Enhanced Chemical Vapour Deposition
DAC = Digital to Analogue Converter
DAS = Data Acquisition System
DC = Direct Current
DCA = Dynamic Contact Angle
DBM = Demineralized Bone Matrix
DLC = a-C:H = Diamond Like Carbon
DMSO = Dimethylsulphoxide
DSP = Data Signal Processor
ECM = Extracellular Matrix
EDS = Energy Dispersive Spectroscopy
EDTA = Ethylene-di-tetra-acetic acid
EGF = Epithelial Growth Factor
ELISA = Enzyme Linked Immuno-Sorbent Assay
EM = Electroforetic Mobility
FAT = Fixed Analyser Transmission
FCS = Foetal Calf Serum

FTIR = Fourier Transform Infra-Red
GPIB = General Purpose Interface Bus
Hela = Henrietta Lacks-cervical carcinoma cell line (the first in-vitro human cell line)
HMDS = Hexamethyldisilaxane
HMEC = Human Microvascular Endothelial Cell
L132 = Human embryonic lungs cell line (Hela-characteristics/contamination)
LASER = Light Amplification by Stimulated Emission of Radiation
LED = Light Emitting Diode
MCDB = Microvascular endothelial cell growth media
MEM = Minimal Essential Media
DMEM = Dulbecco Minimal Essential Media
PPP = Platelet Poor Plasma
MSM = Metal Semiconductor Metal sandwich
MTT = 3-(4, 5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide
N1 = N-DLC film obtained with nitrogen ions bombardment for 1 hour
N1h = N-DLC film obtained with nitrogen ions bombardment for 1.5 hours
N2= N-DLC film obtained with nitrogen ions bombardment for 2 hours
N2h = N-DLC film obtained with nitrogen ions bombardment for 2.5 hours
N-DLC = a-C:H:N = Nitrogen doped Diamond Like Carbon
NEAA = Non-Essential Amino Acid
PBS = Phosphate Buffered Saline
PRP = Platelet Rich Plasma
Ra = Arithmetical Mean Roughness
RF = Radio Frequency
RMS = Root Mean Square
Sccm= Standard cubic centimetre
SD10 = Si-DLC film obtained using TMS flow rate of 10sccm
SD15 = Si-DLC film obtained using TMS flow rate of 15sccm
SD20 = Si-DLC film obtained using TMS flow rate of 20sccm
SD5 = Si-DLC film obtained using TMS flow rate of 5sccm
SEM = Scanning Electron Microscope

Si-DLC = a-C:H:Si = Silicon doped Diamond Like Carbon
SN1 = N-DLC film obtained with nitrogen neutrals bombardment for 1 hour
SN1h = N-DLC film obtained with nitrogen neutrals bombardment for 1.5 hours
SN2 = N-DLC film obtained with nitrogen neutrals bombardment for 2 hours
SN2h = N-DLC film obtained with nitrogen neutrals bombardment for 2.5 hours
SPR = Surface Plasmon Resonance
SW = Silicon wafer (uncoated)
TCPS = Tissue culture polysterene
TMS = Tetramethylsilane
T_R = Room temperature
V79 = Chinese Hamster cell line
WF = Work Function
WR = Web Reference
XPS = X-ray Photoelectron Spectroscopy
ZDOI = Zero Depth of Immersion
σ = Bending strength
θ = Contact Angle
λ = Wavelength

1. Atomic Scale Machining of Surfaces

1.1 Introduction

Molecular dynamic simulations of machining at the atomic scale can reveal a significant amount of information regarding the behavior of machining and grinding processes that cannot be explained easily using classical theory or experimental procedures. This chapter explains how the use of molecular dynamic simulations can be applied to the many problems associated with machining and grinding at the meso, micro, and nanoscales. These include: (a) mechanics of nanoscale machining of ferrous and non-ferrous materials; (b) physics of nanoscale grinding of semiconductor materials; (c) effects of simulating a variety of machining parameters in order to minimize sub-surface damage; (d) modeling of exit failures experienced during machining such as burr formation and other dynamic instabilities during chip formation; (e) simulation of known defects in microstructures using molecular dynamic simulations, statistical mechanical, and Monte Carlo methods; (f) simulation of machining single crystals of known orientation; (g) extremely high speed nanometric cutting; (h) tool wear during machining; and (i) the effects of hardness on the wear of tool and workpiece materials. The nature of wear of the material ahead of the machining and grinding process, the variation of machining forces, and the amount of specific energy induced into the workpiece material using molecular dynamic simulations is discussed in this chapter.

Nanotechnology is the creation and utilization of materials, structures, devices and systems through the control of matter at the nanometer length scale. The essence of nanotechnology is the ability to work at these levels to generate large structures with fundamentally new properties. Although certain applications of nanotechnology, such as giant magnetoresistance (GMR) structures for computer hard disk read head and polymer displays have entered the marketplace, in general nanotechnology is still at a very early stage of development.

The barriers between nanotechnology and the marketplace lie in how to reduce the fabrication cost and how to integrate nanoscale assemblies with functional microscale and macro devices. Therefore, reliable mass production of nanostructures is currently one of the most crucial issues in nanotechnology. The commercialization of nanotechnology has to address the underlying necessities of predictability, repeatability, producibility and productivity in manufacturing at nanometer scale.

Nanometric machining refers to a “top down” nanofabrication approach. To the authors’ knowledge the concept of nanometric machining is more concerned with precision rather than the characteristic size of the product. Therefore, nanometric machining is defined as the material removal process in which the dimensional accuracy of a product can be achieved is 100 nm or less. Nanometric machining can be classified into four categories:

- Deterministic mechanical nanometric machining. This method utilizes fixed and controlled cutting tools, which can specify the profiles of three-dimensional components by a well-defined tool surface. The method can remove materials in amounts as small as tens of nanometers. It includes processes such as diamond turning, micro milling, and nano/micro grinding.
- Loose abrasive nanometric machining. This method uses loose abrasive grits to removal a small amount of material. It consists of polishing, lapping, and honing, etc.
- Non-mechanical nanometric machining comprises processes such as focused ion beam machining, micro-EDM, and excimer laser machining.
- Lithographic method. The method employs masks to specify the shape of the product. Two-dimensional shapes are the main outcome; severe limitations occur when three-dimensional products are attempted [1]. Processes include X-ray lithography, LIGA, and electron beam lithography.

The author believes that mechanical nanometric machining has more advantages than other methods since it is capable of machining complex 3D components in a controllable and deterministic way.

The machining of complex surface geometries is just one of the future trends in nanometric machining, which is driven by the integration of multiple functions in one product. For instance, the method can be used to machine micro moulds/dies with complex geometric features and high dimensional and form accuracy, and even nanometric surface features. The method is indispensable to manufacturing complex micro and miniature structures, components, and products in a variety of engineering materials. This chapter focuses on nanometric cutting theory, methods, and its implementation and application perspectives.

1.2 Theoretical Basis of Nanomachining

The scientific study of nanometric machining has been undertaken since the late 1990s. Much attention to the study has been paid especially with the advancement of nanotechnology [2]. The scientific study will result in the formation of the theoretical basis of nanometric machining, which enables the better understanding of nanometric machining physics and the development of controllable techniques to meet the requirements for nanotechnology and nanoscience.

1.2.1 Cutting Force and Energy

In nanomanufacturing, the cutting force and cutting energy are important issues. They are important physical parameters for understanding cutting phenomena as they clearly reflect the chip removal process. From the point of view of atomic structures, cutting forces are the superposition of the interactions of forces between workpiece atoms and cutting tool atoms. Specific energy is an intensive quantity that characterizes the cutting resistance offered by a material [3]. Ikawa et alia [2], and Luo et alia [4] have acquired the cutting forces and cutting energy by molecular dynamics (MD) simulations. Ikawa et alia [2] have carried out experiments to measure the cutting forces in nanometric machining. Table 1.1 shows the simulation and experimental results in nanometric cutting. Table 1.1 (a) illustrates the linear relationship that exists between the cutting force per width and depth of cut in both simulations and experiments. The cutting forces per width increase with the increment of the depth of cut.

The difference in the cutting force between simulations and experiment is caused by the different cutting edge radii applied in the simulations. In nanometric machining the cutting edge radius plays an important role since the depth of cut is similar in scale. Under the same depth of cut higher cutting forces are required for a tool with a large cutting edge radius compared with a tool with a small cutting edge radius. The low cutting force per width is obviously the result of fine cutting conditions, which will decrease the vibration of the cutting system and thus improve machining stability and will also result in better surface roughness.

A linear relationship between the specific energy and the depth of cut can also be observed in Fig. 1.1. The figure shows that the specific energy increases with a decreasing of depth of cut, because the effective rake angle is different under different depths of cut. In small depths of cut the effective rake angle will increase with the decreasing of depth of cut. Large rake angles result in an increase in specific cutting energy. This phenomenon is often called the 'size effect', which can be clearly explained by material data listed in Table 1.1. According to Table 1.1, in nanometric machining only point defects exist in the machining zone in a crystal. Therefore, the material will need more energy to initiate the formation of an atomic-crack or the movement of an atomic-dislocation. The decreasing of depth of cut will decrease the chance for the cutting tool to meet point defects in the material and will result in increasing the specific cutting energy.

If the machining unit is reduced to 1 nm, the workpiece material structure at the machining zone may approach atomic perfection, hence more energy will be required to break the atomic bonds. Alternatively, when the machining unit is higher than 0.1 μm, the machining points will fall into the distribution distances of some defects such as dislocations, cracks, and grain boundaries. The pre-existing defects will ease the deformation of workpiece material and result in a comparatively low specific cutting energy.

Nanometric cutting is also characterized by the high ratio of the normal to the tangential component in the cutting force [3,4], as the depth of cut is very small in nanometric cutting and the workpiece is

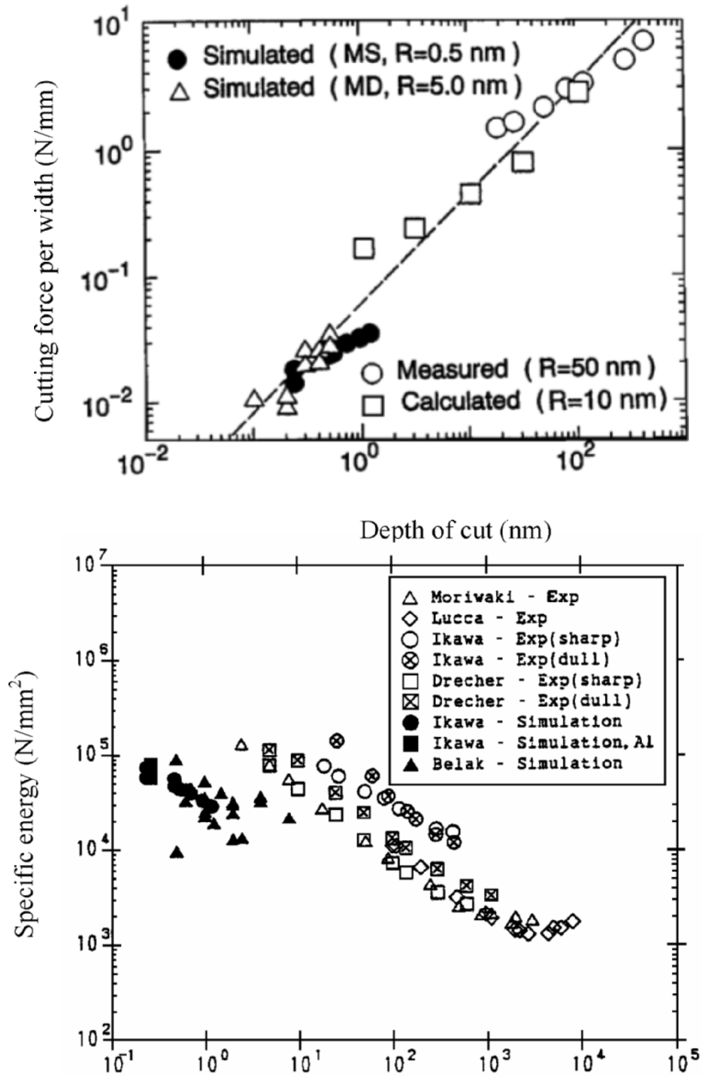
Table 1.1. Material properties under different machining units [5].

	1nm – 0.1 μm	**0.1 μm – 10 μm**	**10 μm – 1 mm**
Defects/Impurities	Point defect	Dislocation/crack	Crack/grain boundary
Chip removal unit	Atomic cluster	Sub-crystal	Multi-crystals
Brittle fracture limit	10^4 J/m^3 - 10^3 J/m^3 Atomic-crack	10^3 J/m^3 - 10^2 J/m^3 Micro-crack	10^2 J/m^3 - 10^1 J/m^3 Brittle crack
Shear failure limit	10^4 J/m^3 - 10^3 J/m^3 Atomic-dislocation	10^3 J/m^3 - 10^2 J/m^3 Dislocation slip	10^2 J/m^3 - 10^1 J/m^3 Shear deformation

mainly processed by the cutting edge. The compressive interactions will thus become dominant in the deformation of the workpiece material, which will therefore result in the increase of friction force at the tool-chip interface with a relatively high cutting ratio.

Usually, the cutting force in nanometric machining is very difficult to measure due to its small amplitude compared with the noise generated (mechanical or electronic) [2]. A piezoelectric dynamometer, or load cell, is used to measure the cutting forces because of their characteristic high sensitivity and natural frequency. Figure 1.2 shows an experimental force measuring system in micromilling process carried out by Dow et alia [6]. The three-axis load cell, Kistler 9251, is mounted in a specially designed mount on the Y-axis of a Nanoform 600 diamond turning machine. A piece of S-7 steel that has been ground flat on both sides is used as the workpiece and secured through the top of the load cell with a bolt preloaded to 30 N. The tool was moved in the +Z direction to set the depth of cut and the workpiece was fed in the +y direction to cut the groove.

The milling tool is mounted in a Westwind D1090-01 air bearing turbine spindle capable of speeds up to 60,000 rpm. The spindle is attached to the Z-axis of the Nanoform 600. To determine the rotational speed of the tool and the orientation of each flute, an optical detector (Angstrom resolver) was used to indicate a single rotation of the spindle by reading a tool revolution marker aligned with one flute. The measured 3D cutting forces under depth of cut of 25 μm, feed rate of 18.75 μm/flute, are of the order of several Newtons.



(a)

(b)

Fig. 1.1. The comparison of results between simulations and experiments: (a) cutting force per width against depth of cut; (b) specific energy against depth of cut [2].

1.2.2 Cutting Temperature

In MD simulations, the cutting temperature can be calculated under the assumption that the cutting energy totally transforms into cutting

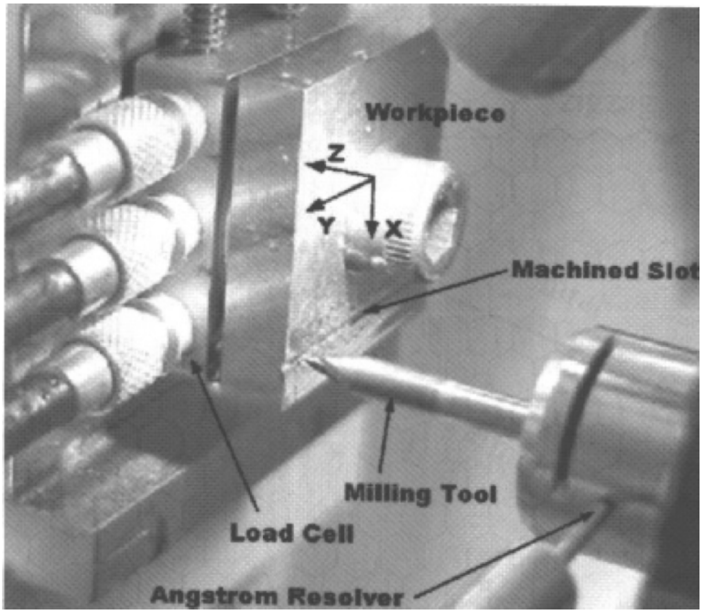


Fig. 1.2. Experimental force measurement system in micro-milling process [6].

heat and results in increasing the cutting temperature and kinetic energy of system. The lattice vibration is the major form of thermal motion of atoms. Each atom has three degrees of freedom. According to the theorem of equi-partition of energy, the average kinetic energy of the system can be expressed as:

$$\bar{E}_k = \frac{3}{2} N k_B T = \sum_i \frac{1}{2} m(V_i^2) \tag{1.1}$$

Where $\bar{E}_k$ is average kinetic energy in equilibrium state, K_B is Boltzmann's constant, T is absolute temperature, and m_i and V_i are the mass and velocity of an atom, respectively. N is the number of atoms.

The cutting temperature can be calculated using the following equation:

$$T = \frac{2\bar{E}_k}{3Nk_B} \tag{1.2}$$

Figure 1.3 shows the variation of cutting temperature on the cutting tool in MD simulation of nanometric cutting of single crystal aluminium [7].

The highest temperature is observed at cutting edge although the temperature at the flank face is also higher than that at the rake face. The temperature distribution suggests that a major source of heat exists at the interface between the cutting edge and the workpiece, and that the heat be conducted from there to the rest of the cutting zone. This is because that most of cutting action takes place at the cutting edge of the tool and the resulting dislocation deformation in the workpiece material will transfer their potential energy into kinetic energy and result in the observed temperature rise. The comparatively high temperature exhibited at the flank face is caused by the friction between the flank face and the workpiece. The released energy due to the elastic recovery of the machined surface also contributes to the incremental increase in temperature at flank face. Although there is friction between the rake face and the chip, the heat will be taken away from the rake face by the removal of the chip.

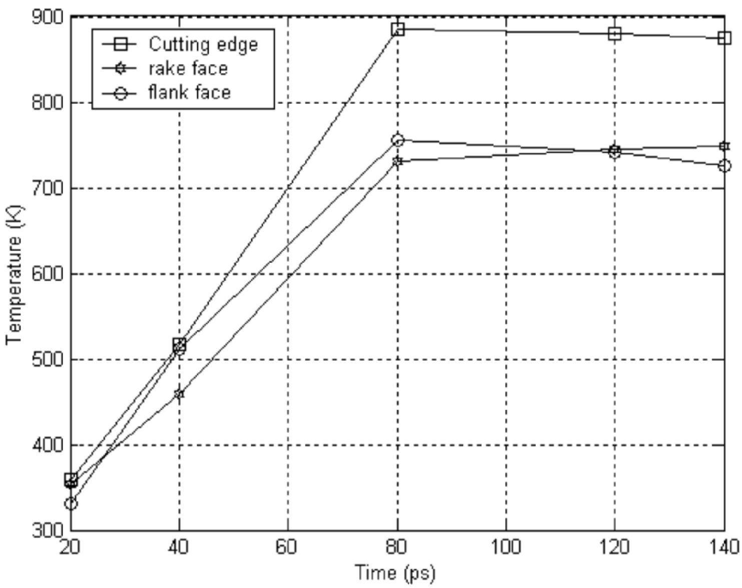


Fig. 1.3. Cutting temperature distribution of cutting tool in nanometric cutting (cutting speed = 20 m/s, depth of cut = 1.5 nm, cutting edge radius = 1.57 nm) [7].

Therefore, the temperature at tool rake face is lower than that at the tool cutting edge and tool flank face. The temperature value shows that the cutting temperature in diamond machining is quite low in comparison with that in conventional cutting, due to low cutting energy in addition to high thermal conductivity of diamond and the workpiece material. The cutting temperature is considered to govern the wear of a diamond tool as shown in the MD simulation study by Cheng et alia [8]. In-depth experimental and theoretical studies are needed to find out the quantitative relationship between cutting temperature and tool wear although there is considerable evidence of chemical damage on the surface of diamond in which increases in temperature tends to plays a significant role [8].

1.2.3 Chip Formation and Surface Generation

Chip formation and surface generation can be simulated by MD simulations. Figure 1.4 shows an MD simulation of a nanometric cutting process on single crystal aluminium [7]. From Fig. 1.4(a) it is shown that after the initial plough of the cutting edge the workpiece, atoms are compressed in the cutting zone near to the rake face and the cutting edge. The disturbed crystal lattices of the workpiece and even the initiation of dislocations can be observed in Fig. 1.4(b). Figure 1.4(c) shows the dislocations have piled up to form a chip. The chip is removed with the unit of an atomic cluster as shown in Fig. 1.4(d). Lattice disturbed workpiece material is observed on the machined surface.

Based on the visualisation of the nanometric machining process, the mechanism of chip formation and surface generation in nanometric cutting can be explained. Owing to the ploughing of the cutting edge, the attractive force between the workpiece atoms and the diamond tool atoms becomes repulsive. Because the cohesion energy of diamond atoms is much larger than that of Al atoms, the lattice of the workpiece is compressed. When the strain energy stored in the compressed lattice exceeds a specific level, the atoms begin to rearrange so as to release the strain energy. When the energy is not sufficient to perform the rearrangement, some dislocation activity is generated. Repulsive forces between compressed atoms in the upper

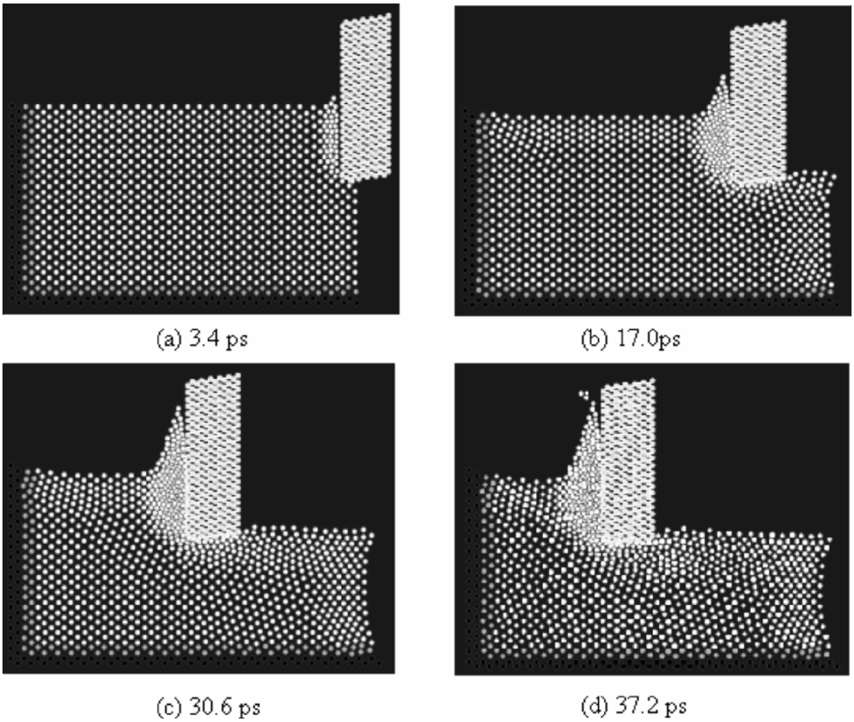


Fig. 1.4. MD simulations of the nanometric machining process (Cutting speed = 20m/s, depth of cut = 1.4 nm, cutting edge radius = 0.35 nm) [7].

layer and the atoms in the lower layer are increasing, so the upper atoms move along the cutting edge, and at the same time the repulsive forces from the tool atoms cause the resistance for the upward chip flow to press the atoms under the cutting line. With the movement of the cutting edge, some dislocations move upward and disappear from the free surface as they approach the surface.

This phenomenon corresponds to the process of chip formation. As a result of the successive generation and disappearance of dislocations, the chip seems to be removed steadily. After the passing of the tool, the pressure at the flank face is released. The layers of atoms move upwards and result in elastic recovery, so that the machined surface is generated.

The conclusion can therefore be drawn that chip removal and machined surface generation are, in nature, dislocation slip motion inside the workpiece material grains. In conventional cutting, dislocations