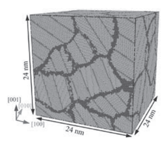
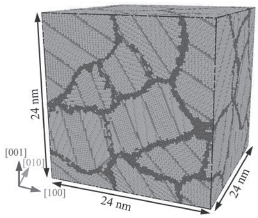
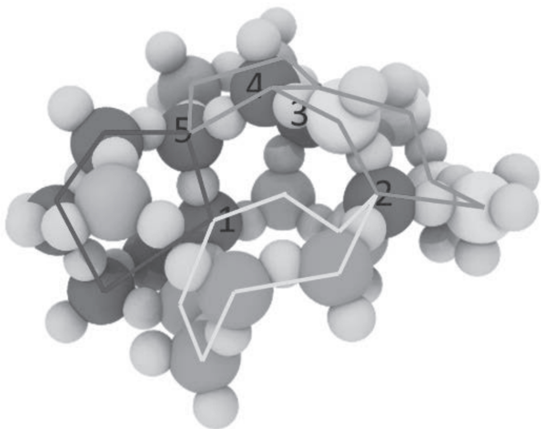
MOLECULAR DYNAMICS FOR TRIBOLOGY



MOLECULAR DYNAMICS FOR TRIBOLOGY





Liang Fang
Xiamen University Tan Kah Kee College, China

World Scientific

NEW JERSEY • LONDON • SINGAPORE • BEIJING • SHANGHAI • HONG KONG • TAIPEI • CHENNAI • TOKYO

Published by

World Scientific Publishing Co. Pte. Ltd.
5 Toh Tuck Link, Singapore 596224
USA office: 27 Warren Street, Suite 401-402, Hackensack, NJ 07601
UK office: 57 Shelton Street, Covent Garden, London WC2H 9HE

Library of Congress Cataloging-in-Publication Data
Names: Fang, Liang (Professor on mechanical engineering) author
Title: Molecular dynamics for tribology / Liang Fang,
Xiamen University Tan Kah Kee College, China.
Description: New Jersey : World Scientific, [2026] | Includes bibliographical references and index.
Identifiers: LCCN 2025011023 | ISBN 9789819812943 hardcover |
ISBN 9789819812950 ebook for institutions | ISBN 9789819812967 ebook for individuals
Subjects: LCSH: Microelectromechanical systems--Simulation methods |
Molecular dynamics--Simulation methods
Classification: LCC TK7875 .F36 2025 | DDC 621.38101/13--dc23/eng/20250612
LC record available at https://lccn.loc.gov/2025011023

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library.

摩擦磨损的分子动力学
Originally published in Chinese by China Machine Press Co., Ltd.

For any available supplementary material, please visit
https://www.worldscientific.com/worldscibooks/10.1142/14307#t=suppl

Desk Editors: Murali Appadurai/Steven Patt

Typeset by Stallion Press
Email: enquiries@stallionpress.com

Printed in Singapore

Preface

With the increasing maturity of Micro-Electro-Mechanical Systems (MEMS) applications and the growing demand for large-scale integrated circuit manufacturing, the tribological issues that arise during manufacturing and application have garnered significant attention from scholars both domestically and internationally in recent years. The tribological research within these two domains falls under the field of nanotribology. In terms of applications, scholars have primarily focused on reducing friction and wear, whereas in manufacturing, the interest lies in the scientific utilization and control of friction and wear. A quintessential example is Chemical Mechanical Polishing (CMP) in chip manufacturing, where the goal is to maximize the material removal rate (MRR) while minimizing defects, which is contrary to the objective in applications where minimizing material wear is desired.

The rapid development of nanotribology research is closely tied to advances in modern microscopic detection technologies, such as Scanning Electron Microscopy (SEM), High-Resolution Transmission Electron Microscopy (HRTEM), X-ray Photoelectron Spectroscopy (XPS), Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM), and Nanoindentation Instruments (NI). Among these, the novel nanoindentation instruments, which integrate

AFM capabilities, not only facilitate nanoindentation tests but also enable nano-scratch tests, yielding precise measurements of mechanical behaviors at the nanoscale or microscale, such as indentation hardness, elastic modulus, yield strength, and fracture toughness. Some advanced nanoindentation devices can also conduct tests on micro/nano-scale materials, such as compression, tension, fracture, fatigue, friction, and wear, significantly advancing the field of nanotribology. Theoretically, the development of molecular simulation techniques, particularly molecular dynamics simulation software, has undoubtedly provided a catalyst for nanotribology research. These simulations can overcome the limitations of real nanoscale experiments by using large-scale parallel computing to simulate nanoscale friction and wear processes. The collaboration between molecular simulation theory and modern microscopic detection technologies has extended our understanding to the atomic and molecular levels, making cross-scale research truly feasible.

Like traditional tribology, nanotribology involves friction, wear, and lubrication and is an interdisciplinary field related to mathematics, physics, chemistry, mechanics, mechanical engineering, crystallography, and materials science. This book focuses on a highly specialized area within this broad field, namely, the use of molecular dynamics simulation software LAMMPS to simulate the nanoscale wear processes of various materials, aiming to derive general principles that could lay a foundation for practical applications in this domain.

Chapter 1 provides a brief overview of the development and application value of molecular dynamics. Chapter 2 outlines the principles, potential functions, and simulation tools of molecular dynamics. Chapter 3 begins with the theory and experiments of nanoindentation, followed by a discussion of the regularities observed in the nanoindentation of single-crystal copper and single-crystal silicon using molecular dynamics simulation. The final section of this chapter discusses the uniaxial tensile behavior of single-crystal nanowires, proposing the idea that material scale significantly influences material properties. Chapter 4 systematically explores the simulated experiments and findings on the nanoscale two-body and three-body abrasive wear of single-crystal copper under air lubrication, followed by a discussion on the nanoscale abrasive wear of single-crystal silicon. It highlights that one of the key differences between nanoscale and macroscopic abrasive wear is the need to account for the elastic recovery of the worn surface, leading to an improved criterion for distinguishing sliding and rolling of ellipsoidal abrasives at the nanoscale. Chapter 5 analyzes the behavior of single-crystal copper under nanoindentation, two-body, and three-body abrasive wear in the presence of a water film, extending the criteria for abrasive rolling and sliding to conditions with water lubrication. The presence of a water film reduces the friction coefficient and affects the material removal rate. Chapter 6 directly addresses the CMP process, systematically discussing the nanoindentation and wear behavior of single-crystal silicon surfaces covered with an amorphous silica film and analyzing the material removal mechanisms in the presence of a water film. It also explores the wear process using non-rigid abrasives, finding that non-rigid abrasives result in higher material removal efficiency and better surface quality of single-crystal silicon, with no defects in the substrate. In Chapter 7, the author systematically studies the deformation behavior of nanocrystalline copper using molecular dynamics and, combined with phase field modeling, constructs a more realistic polycrystalline model. This model quantitatively analyzes the movement of grain boundaries and the evolution of twinning, providing theoretical support for the rational design of crystal structures in the future.

This book is a continuation of my previous monograph on “Abrasive Wear” which has been published by China Science Publishing & Media LTD. The content presented here summarizes over ten years of the author’s latest research. The main chapters and computational data were contributed by my doctoral students, including Dr. Jiapeng Sun (Associate Professor at Hohai University), Dr. Junqin Shi (Associate Professor at Northwestern Polytechnical University), Dr. Juan Chen (Associate Professor at Taiyuan University of Science and Technology), Dr. Meng Zhang (Postdoctoral Fellow at the University of Tokyo), and outstanding master’s student Mr. Xiangzheng Zhu (Mindray Bio-Medical Electronics Co., Ltd.). I would like to extend my heartfelt thanks to all my students, especially Dr. Meng Zhang, who made significant contributions to the typesetting, organization, and writing of Chapters 1, 2, and 7. I also express my gratitude to the National Natural Science Foundation of China for funding the publication of this book (Project No. 51375364: Nanotribology of Three-Body Abrasive Wear in MEMS). I take this opportunity to thank my colleagues and other graduate students in my research group for their strong support during my research work. I am also grateful to all my friends, family, and relatives who have supported me. This book was completed at Xiamen University Tan Kah Kee College.

Errors in the book are inevitable, and I hope readers will understand and provide constructive feedback to help the author make corrections in future editions.

About the Author

Liang Fang is a Professor at Xiamen University Tan Kah Kee College. Before his retirement, he was a Professor at the State-Key Laboratory for Mechanical Behavior of Materials (SKL-MBM) at Xi'an Jiaotong University. He is the Editorial board member of the journal *Wear* published by Elsevier Group PLC and the journal *Lubrication Science* published by John Wiley & Sons, Inc. He is the recipient of the Outstanding Science and Technology Worker Award from the Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, and the Advanced Organizational Work Award from the Chinese Mechanical Engineering Society. His research interests are in molecular dynamics in wear process and the modeling and computer simulation of abrasive wear processes in materials. He has published about 209 papers with H-Index 34.

Contents