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Review of Molecular Dynamics Simulations in Semiconductor Material Engineering

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Abstract—*Molecular dynamics (MD) simulation has become an indispensable tool in the research and development of semiconductor nanomaterials, playing a crucial role in modern semiconductor fabrication technologies. This approach not only enables the optimization of semiconductor materials but also offers in-depth insights into their fundamental atomic-scale properties, thereby enhancing the performance and reliability of semiconductor devices. In the current landscape of the semiconductor industry, where demands for quality and performance continue to rise, MD simulations serve as a critical method for designing, optimizing, and refining material processing techniques. This review presents a comprehensive analysis of state-of-the-art MD simulation methods applied in semiconductor nanomaterial fabrication, with a particular emphasis on mechanical mechanisms and microstructural [1] transformations during processing. Advanced techniques such as surface machining, ion implantation, laser processing, and vibration-assisted machining can be effectively optimized using MD simulations, which help elucidate the mechanical, thermodynamic, and microstructural changes involved in these processes. Despite its advantages, MD simulation faces several challenges, including the calibration of interatomic potentials, accurate prediction of chemical reactions under extreme processing conditions, and the simulation of complex nanoscale systems. To overcome these limitations, this study also explores recent advances, such as the integration of MD with emerging computational techniques like machine learning, to improve accuracy and predictive capability. The paper concludes by outlining future research directions, highlighting the continuous evolution of MD simulation and its potential integration with advanced technologies such as multiscale modeling and quantum-classical hybrid simulations, aiming to further enhance semiconductor manufacturing and expand the application of these materials in high-tech industries, ultimately contributing to the ongoing innovation in the global semiconductor field.*

Keywords— *Molecular dynamics (MD), nano-polishing, nano-cutting, SiC, GaN.*

I. INTRODUCTION

In the context of rapid development in electronics and microelectronics, semiconductor materials play a crucial role in driving modern technological advancements. From basic applications in integrated circuits to consumer electronics, communication systems, and high-power devices, semiconductors have become an indispensable foundation. Silicon (Si), as a traditional semiconductor material, has significantly contributed to the development of devices such as MOSFETs and IGBTs[2, 3]. However, with increasing demands for performance, thermal resistance, and high-power handling capability, new-generation semiconductor materials such as silicon carbide (SiC), gallium nitride (GaN), and gallium oxide (Ga_2O_3) have attracted significant attention due to their superior properties, including high thermal stability, large breakdown voltages, and wide bandgaps[4, 5]. These properties open up opportunities for applications in harsh environments and high-power systems[6, 7].

However, the machining of these semiconductor materials faces numerous challenges due to their physical characteristics, such as high hardness and brittleness, which make the processing particularly difficult at the nanoscale. For example, SiC exhibits high hardness and brittleness, which lead to issues such as microcrack formation, structural distortion, and phase transformation on both the surface and subsurface layers[8]. These defects reduce the performance and lifespan of electronic devices and complicate the optimization of manufacturing processes. GaN also faces similar challenges, especially in single-crystal growth, where lattice mismatch between the substrate and the epitaxial layer results in lattice defects and undesirable crystallization, affecting the structural integrity of the material[9].

To address these challenges, high-precision surface machining methods such as chemical mechanical polishing (CMP) have been extensively studied and applied. CMP enables surface finishing with low roughness and minimal surface damage, but it still has limitations in terms of material removal rate (MRR) and operational cost. To overcome these limitations, more advanced methods such as electrochemical mechanical polishing (ECMP), photocatalytic chemical mechanical polishing (PCMP), plasma-assisted polishing (PAP), and catalyst-referred etching (CARE) have been developed to optimize processing and improve surface quality, particularly in the fabrication of materials such as SiC and GaN[10].

In this scenario, molecular dynamics (MD) simulation has emerged as a significant instrument for the exploration and advancement of semiconductor materials. MD allows the analysis of physical and chemical processes at the atomic scale, helping to reconstruct and predict material properties as well as processing mechanisms. By using MD, researchers can better understand structural, mechanical, and electronic transformations of semiconductor materials during machining processes such as cutting, scratching, and deformation, thereby optimizing material processing strategies.

In this study, LAMMPS is selected as the primary simulation tool due to its flexibility in simulation parameter setup, system relaxation, execution, and data output. Choosing an appropriate interatomic potential is a critical factor for accurately simulating complex physical and chemical processes such as plastic deformation, structural failure, phase

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transitions, or surface chemical reactions. Popular potentials in semiconductor material simulations include Tersoff, Stillinger-Weber (SW), and ReaxFF, each with its own advantages and limitations, suitable for specific materials and processing conditions[11].

MD not only provides deep insights into the structure and mechanics of semiconductor materials but also enables the simulation and analysis of factors affecting processing performance, including temperature, stress, and nanostructures. Recent studies have employed MD to investigate processes such as phase transformation, amorphization, and crack propagation in semiconductor materials like SiC, GaN, and Ga_2O_3, offering detailed models of material structure evolution under various processing conditions[12]. Additionally, MD has been used to analyze emerging phenomena in the semiconductor field, such as the quantum anomalous Hall effect in transition-metal-doped silicene, opening up new potential for innovative processing technologies and the development of semiconductor devices with superior electronic properties[13].

This paper provides a comprehensive overview of the application of molecular dynamics simulations in the study and fabrication of semiconductor materials[13]. The study focuses on evaluating MD models and methodologies, analyzing advanced processing techniques, and proposing future research directions to optimize semiconductor material processing[14]. By using MD to elucidate nanoscale fabrication mechanisms and optimize processing strategies, this research contributes to improving the performance and reliability of semiconductor devices, while also opening new prospects for sustainable development and continuous innovation in the semiconductor industry[15].

II. Simulation Methods and Machining Enhancements

2.1. Simulation Techniques for Nanoscale Processes

In the fabrication and processing of semiconductor materials, nanoscale mechanical techniques-including nano-scratch, nano-indentation, nano-cutting, and nano-polishing-play a pivotal role in analyzing the mechanical behavior, deformation mechanisms, and microstructural evolution of materials under localized stress[1, 16]. These processes, when implemented experimentally, allow for the quantitative evaluation of key parameters such as hardness, elastic modulus, adhesion, and friction coefficient, as well as the identification of micro-damage forms such as microcracks, crystal lattice defects, and surface deformation layers. However, to gain deeper insight into the underlying physical mechanisms and to optimize processing conditions at the atomic scale, the integration of Molecular Dynamics (MD) simulation has become increasingly essential.

Specifically, nano-scratch simulations enable detailed tracking of groove formation and wear behavior when a probe or hard abrasive particle slides across the crystal surface under a defined load. This approach helps clarify mechanisms such as lattice fracture, amorphous layer formation, and microstructural disruptions-factors that critically determine the surface durability of hard materials like GaN or SiC.

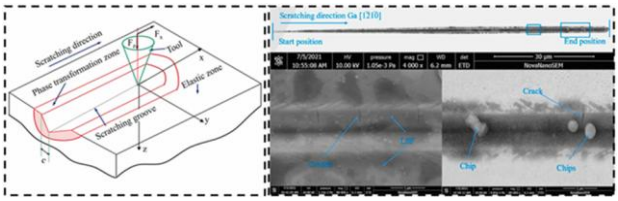

Fig. 1. Schematic and experimental setup of the scratching process[17, 18].

Similarly, the nano-indentation technique, which simulates the process of pressing a sharp indenter into the surface of a material, allows for the investigation of stress and strain distribution within the loaded region, while also elucidating the initiation of dislocations, amorphization, or localized phase transformations. This technique provides deep insights into the material's hardness and elastic recovery behavior under micro-scale loading conditions.

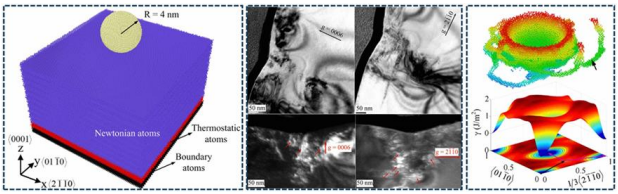

Fig. 2. Nanoindentation process and analysis [19].

In nano-cutting simulations, the material removal process is reproduced at the atomic scale under conditions analogous to those in real-world micro-turning or micro-milling operations. This enables the evaluation of the effects of cutting speed, cutting depth, and tool geometry on deformation mechanisms, material damage, and the resulting surface quality. Such simulations aid in the optimization of machining parameters to minimize defects and enhance the surface integrity of semiconductor materials.

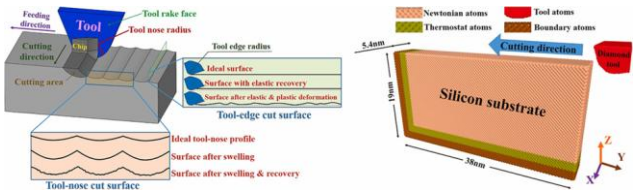

Fig. 3. Schematic diagram of different surface deformations during nano-cutting [20].

Finally, nano-polishing simulation plays a particularly important role in analyzing the multidimensional interactions among abrasive particles, the material surface, and the surrounding environment, where factors such as friction, temperature, and chemical reactions occur simultaneously. This process not only provides quantitative data such as material removal rate (MRR), polishing force, abrasive wear, and surface scratch levels, but also helps unravel the fundamental mechanisms that influence the polishing efficiency of ultra-hard materials such as SiC or GaN[21-23].

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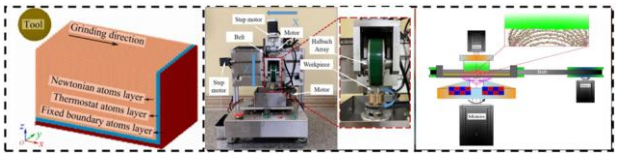

Fig. 4. MD simulation model and nano-milling/polishing experimental setup [24-26].

Overall, the application of MD simulations in nanoscale mechanical machining processes not only enables accurate reproduction of physical phenomena at the atomic level but also offers great potential for tailoring machining strategies to optimize surface quality, extend device lifespan, and enhance the performance of next-generation semiconductor components.

2.2. Selection and Application of Potential Functions

In molecular dynamics (MD) simulations, the potential function, also known as the interatomic potential, plays a crucial role in determining the interaction forces between atoms, thereby directly influencing the simulation results. Choosing an appropriate potential function is key to accurately simulating complex physical and chemical processes such as plastic deformation, structural breakage, phase transitions, or surface chemical reactions. The accuracy of both the kinetic and thermodynamic results can be strongly affected by this choice, making it essential for simulating atomic-level phenomena.

Common Potential Functions in Semiconductor Material Simulations:

EAM (Embedded Atom Method): Suitable for metals, EAM describes the energy of the system through a combination of pairwise atomic energy and embedding energy into the electron density around the atoms. While EAM is not suitable for covalently bonded semiconductor materials, it is very useful in simulations of metal-semiconductor interfaces or mixed materials.

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho_{\alpha\beta}\left(r_{ij}\right)\right)+\frac{1}{2}\sum_{j\neq i}\varnothing_{\alpha\beta}\left(r_{ij}\right) \quad (1)$$

In this expression, ρ represents the electron density contributed by the neighboring atom j (of a certain element) at the position of atom i (of a different element). This formula follows the same structure as the previously mentioned EAM formula, except that ρ is now a function specifically dependent on the elements of both atoms i and j. As a result, different elements may contribute differently to the total electron density at a given atomic position, depending on the elemental nature of the atoms at that position.

Tersoff Potential: This is a commonly used potential for covalent systems such as silicon, carbon, and III-V compounds like GaAs and GaN. Tersoff allows for the simulation of bond angle changes and crystal lattice breakage/shearing reactions during mechanical processing at the nano level. However, this potential is not flexible enough to model complex chemical reactions, especially those involving changes in valence states.

$$E=\sum_i\sum_{j\rangle i} f_C\left(r_{ij}\right)\left[\, f_R\left(r_{ij}\right)+b_{ij}\, f_A\left(r_{ij}\right)\right] \quad (2)$$

Where Fα is the embedding energy function, which depends on the local electron density, $f_R\left(r_{ij}\right)$ and $f_A\left(r_{ij}\right)$ represents the electron density contributed by atom j at the position of atom i, b_{ij} is the pair potential between atoms i and j. The Embedded Atom Method (EAM) potential is well-suited for simulating metallic systems, where the embedding energy plays a crucial role in accurately describing the interatomic bonding.

Stillinger–Weber (SW): A straightforward yet efficient variant for silicon-oriented systems, SW is adept at modeling the creation and rupture of bonds during processes such as annealing, fracture, or nano-indentation. However, like Tersoff, SW is not suitable for simulating dynamic chemical reactions.

$$E_{total}=\sum_{i\langle j}V_2\left(r_{ij}\right)+\sum_{i\langle j\langle k}V_3\left(r_{ij},r_{ik},\theta_{ijk}\right) \quad (3)$$

Where $V_2\left(r_{ij}\right)$ is the two-body term, which describes the interaction between two atoms, $V_3\left(r_{ij},r_{ik},\theta_{ijk}\right)$ is the three-body term, which depends on the angle between three atoms and helps capture the structural characteristics of the material. The Stillinger–Weber (SW) potential is suitable for simulating bond formation and breaking processes during thermal treatment, fracture, or nano-indentation.

ReaxFF (Reactive Force Field): This is an advanced reactive force field that allows the simulation of processes involving chemical reactions, including bond formation and breaking, phase transitions, and multi-element interactions. ReaxFF is particularly useful in simulating semiconductor material processing under harsh conditions such as high temperatures, large stresses, or reactive environments, such as in chemical-mechanical polishing (CMP), plasma treatment, or etching processes. Its ability to simulate processes like oxidation, corrosion, or interactions with catalysts makes ReaxFF an ideal choice for multiphysics studies.

$$E_{total}=E_{bond}+E_{over}+E_{under}+E_{val}+E_{pen}+E_{tors}+E_{conj}+E_{vdW}+E_{Coulomb} \quad (4)$$

In this context, E_{bond} is the bond energy, E_{over} and E_{under} are penalty energies for over-coordination and under-coordination, respectively, E_{val}, E_{pen}, E_{tors}, E_{conj} represent energy contributions associated with bond angles, penalties, torsion, and conjugation, respectively. E_{vdW} and $E_{Coulomb}$ are the van der Waals and Coulombic interaction energies. The ReaxFF potential is particularly useful for simulating material processing in semiconductors under extreme conditions such as high temperatures, large mechanical stresses, or reactive environments.

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The choice of an appropriate potential function depends on the type of material being studied, the specific processing conditions, and the physical or chemical phenomena that need to be simulated. In semiconductor material processing studies, such as for Si, GaN, or SiC, research often combines multiple potential functions to analyze different aspects of the process: Tersoff for simulating nano-cutting and network structure, SW for analyzing thermal deformation, and ReaxFF for investigating chemical corrosion or plasma polishing phenomena.

Finally, to ensure accuracy and stability in simulations, potential functions must be calibrated for the specific atomic system in question. Validating the potential function through experimental data or first-principles calculations is crucial. Comparing results from different potential functions helps assess the reliability and correctness of the chosen simulation model.

2.3. Machining support methods

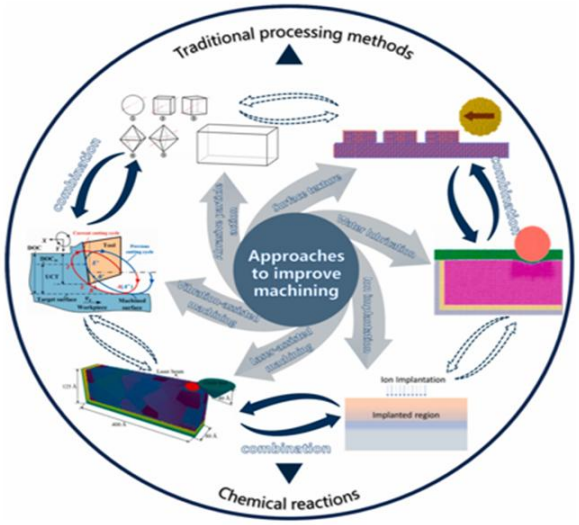

Fig. 5. Six typical improvement methods and correlations [27-32].

For semiconductor materials with high hardness and brittleness, such as SiC, GaN, or Ga_2O_3, traditional machining methods often do not meet the requirements for precision and surface quality. Therefore, supporting methods such as CMP, PCMP, PAP, and CARE are increasingly applied to improve processing performance, reduce micro-damage, and optimize surface conditions. Molecular dynamics (MD) simulations play a crucial role in analyzing the mechanistic behavior of these methods at the atomic level.

CMP (Chemical Mechanical Polishing): This method combines abrasion and chemical reactions, helping to create smooth surfaces with minimal damage. MD supports the analysis of cutting mechanisms, grinding, and subsurface damage development.

PCMP (Photocatalytic Chemical Mechanical Polishing): Using photocatalysts such as TiO_2 and UV light to enhance oxidation efficiency, MD simulations, combined with ReaxFF, help understand the process of bond formation and breaking.

PAP (Plasma-Assisted Polishing): This method combines plasma and soft grinding to remove material with low force. MD allows the study of ion-material interactions, phase transitions, and the creation of network defects.

CARE (Catalytic Etching): Using metal catalysts to promote dissolution reactions without mechanical grinding, MD describes the propagation of reactions and the relationship between crystal structure and etching rates.

Additionally, methods such as ultrasonic machining or femtosecond laser polishing also help reduce cutting forces and improve surface quality. In these processes, MD simulations aid in describing phenomena such as micro-cracking, melting, and crystal transformation. The integration of MD into the study of supporting machining methods provides a scientific foundation for optimizing modern semiconductor material processing and enhancing device reliability.

III. Challenges and Future Prospects

Molecular dynamics (MD) simulations have proven to be essential in analyzing and optimizing semiconductor material processing. However, this method still faces several significant challenges that must be addressed to enhance its practical industrial applications. One of the prominent issues is the scale effect, as traditional MD simulations can only handle systems ranging from several hundred thousand to a few million atoms, corresponding to nanometer-sized scales, with simulation times limited to nanoseconds. This creates a stark contrast with actual semiconductor machining processes, which occur at micrometer to millimeter scales and last much longer. Therefore, expanding the scale of MD simulations or integrating them with multi-scale modeling approaches is an important research direction to address this issue.

Additionally, limitations in computational resources are a critical factor. MD simulations require substantial computational power, especially when using complex potentials like ReaxFF to model chemical reactions related to bond formation and breaking. Optimizing algorithms, improving parallel computation performance, and leveraging supercomputing power are necessary solutions to enhance the practical application of MD in material research.

The accuracy of interatomic potentials plays a crucial role in determining the reliability of simulation results. The choice of an appropriate potential depends not only on the material type but also on simulation boundary conditions such as temperature, pressure, stress, and the type of reaction. However, currently, not all material systems have well-calibrated potentials available. Therefore, the development and validation of new potentials, especially those that can accurately describe heterogeneous material systems or complex structural transformation processes, remain an actively advancing research area.

Particularly, simulating chemical reactions under extreme thermal-mechanical conditions, such as those encountered in CMP, plasma, or catalytic etching processes, requires potentials capable of describing dynamic bond reformation, such as ReaxFF. However, the reliability and comprehensive simulation capabilities remain limited, especially when

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simultaneously modeling multiple interacting factors, including chemistry, mechanics, and thermodynamics.

Looking ahead, the advancement of quantum-classical hybrid models, including quantum mechanics/molecular mechanics (QM/MM), is anticipated to be vital in combining the high accuracy of quantum simulations with the scalability and effectiveness of classical approaches. These hybrid approaches enable more precise descriptions of localized chemical reactions within larger material systems, thereby enhancing the predictive capability of simulations under realistic processing and machining conditions.

In parallel, the integration of machine learning (ML) and artificial intelligence (AI) into the development of interatomic potentials, simulation data analysis, and configuration optimization is becoming a prominent trend. Machine learning models, such as Neural Network Potentials (NNP) or Gaussian Approximation Potentials (GAP), show the potential to accurately reproduce potential energy surfaces with nearly the same accuracy as DFT calculations but at much lower computational costs. This opens up the possibility for simulating larger systems over longer timescales and with greater complexity.

Finally, strong collaboration between academia and industry is essential to transfer the research outcomes of MD simulations into real-world production. Simulation models need not only to ensure high accuracy but also to meet product requirements, technological processes, and integration with existing design-manufacturing systems. Interdisciplinary collaborations between materials scientists, semiconductor engineers, and data experts will play a key role in driving digital transformation and modernizing the microelectronics industry.

IV. Conclusion

Molecular dynamics (MD) simulations have become essential in the exploration and enhancement of semiconductor materials, particularly within the realm of microelectronics technology, which increasingly requires exceptional precision and optimization of processes at the atomic scale. Thanks to its ability to simulate in detail processes such as mechanical deformation, structural phase transitions, chemical reactions, and atomic interactions under complex thermo-mechanical conditions, MD not only helps clarify the underlying mechanistic chemistry and mechanics but also significantly contributes to enhancing processing efficiency and material surface quality.

The application of advanced simulation techniques such as nano-scratching, nano-cutting, and polishing, combined with appropriate potentials like ReaxFF and Tersoff, enables the accurate reproduction of real-world machining processes. This allows for the quantitative analysis and optimization of parameters such as frictional forces, micro-damage, material removal mechanisms, and crystal effects, thereby improving the ability to predict and control the production process.

However, to fully exploit the potential of MD simulations, several challenges remain, such as limitations in simulation scale, the accuracy of interatomic potentials, and the ability to model interdisciplinary phenomena. In this context, the integration of machine learning, artificial intelligence, and quantum-classical hybrid models will open up opportunities for the development of next-generation simulation tools with higher accuracy and broader industrial applications.

Moreover, strong collaboration between the academic research community and the semiconductor industry is a key factor in translating simulation results into practical technological solutions. In the future, MD simulations will not only be a research tool but also a platform that supports the design, optimization, and control of modern semiconductor processing techniques, aiming for sustainable development, efficiency, and continuous innovation in the semiconductor industry-one of the most important and strategic industries today.

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