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Simulation of silicon machining with molecular dynamics

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Abstract

When machining brittle materials at microscales, it is possible to achieve cutting in a ductile mode. However, escalating the depth of cut to a critical threshold induces a transition from ductile to brittle behavior in the material removal process. This shift towards brittle machining is closely linked to phase changes within the material. This research simulates the alterations in phase transitions during the machining of silicon with a simulated Berkovich indenter. Utilizing the Tersoff potential to model atomic-level interactions, the study highlights the movement of silicon particles in a system enhancing the durability and manufacturing efficiency of semiconductor devices. It also examines silicon's response to mechanical stress, focusing on the phase transitions crucial for the success of the machining process. Through detailed analysis, this work deepens the understanding of silicon's mechanical behavior at the nanoscale, making a substantial contribution to the fields of materials science and engineering. The application of nanoindentation techniques and simulations via the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) provides valuable insights into the nanoscale mechanical properties of silicon, thereby paving the way for future advancements in materials science and engineering.

Resumo

Ao usinar materiais frágeis em microescalas, é possível alcançar um corte em modo dúctil. No entanto, aumentar a profundidade de corte até um limiar crítico induz a uma transição de comportamento dúctil para frágil no processo de remoção do material. Essa mudança em direção à usinagem frágil está intimamente ligada a alterações de fase dentro do material. Esta pesquisa simula as modificações nas transições de fase durante a usinagem de silício com um indentador Berkovich simulado. Utilizando o potencial de Tersoff para modelar interações em nível atômico, o estudo destaca o movimento de partículas de silício através de um sistema, auxiliando o entendimento para a melhoria da durabilidade e eficiência de fabricação de dispositivos semicondutores. Também examina a resposta do silício ao estresse mecânico, focando nas transições de fase cruciais para o sucesso do processo de usinagem. Por meio de uma análise detalhada, este trabalho aprofunda o entendimento do comportamento mecânico do silício na nanoescala, contribuindo substancialmente para os campos da ciência e engenharia de materiais. A aplicação de técnicas de nanoindentação e simulações por meio do Simulador Massivamente Paralelo de Átomos/Moléculas em Larga Escala (LAMMPS) fornece percepções valiosas sobre as propriedades mecânicas do silício na nanoescala, abrindo caminho para futuros avanços na ciência e engenharia de materiais.

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Contents

List of Figures

List of Tables

List of Abbreviations

DWS	Diamond wire sawing
IWF	Institut für Werkzeugmaschinen und Fertigung
LAS	Loose abrasive slurry sawing
MWS	Multi-wire sawing
MD	Molecular dynamics
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
SEMI	Semiconductor Equipment and Materials International

List of Symbols

Symbol	Unit	Description
E_{ij}	[eV]	Energy potential between a pair of atoms *i* and *j*.
A_{ij}	[eV]	Attraction parameter for the force between atoms.
B_{ij}	[eV]	Repulsion parameter for the force between atoms
λ_{ij}	[Å^{-1}]	Decay parameter for the attraction force
μ_{ij}	[Å^{-1}]	Decay parameter for the repulsion force
r_{ij}	[Å]	Distance between atoms *i* and *j*
ζ	[-]	Coordination function
β	[Å^{-n}]	Fitting parameter
f_c	[-]	Cutting function

Introduction

1.1 Motivation

While there has been notable advancement in the comprehension of silicon's behavior, particularly in the context of its applications in manufacturing and technological processes, a considerable gap remains in the understanding at the molecular level. The bulk of existing research has concentrated on the overall or macroscopic properties of silicon, atomistic behaviors that occur under the influence of external forces and displacements, areas where MD simulations could provide significant insights. The importance of delving into these minute, atomic-scale dynamics cannot be overstated. Such investigations are crucial for unlocking the complexities of silicon processing, enhancing its performance of applications, and understanding the intricate ways in which silicon atoms respond to different types of situations. The motivation for this research was the necessity for a deeper, more systematic exploration of silicon's atomistic behaviors through MD simulations, particularly in scenarios that are relevant to the processing and application of silicon. This approach not only promises to fill the existing knowledge gap but also to propel forward the understanding and optimization of silicon-based materials.

1.2 Related Work

Molecular dynamics (MD) simulations have become a cornerstone in the study of material removal at the nanoscale, providing significant insights into the optimization of the wire saw machining process for silicon. These simulations have been instrumental in shedding light on the complexities of tool wear, the nuances of stress distribution during nanoindentation, and their collective impact on surface quality. By mirroring the parameters and conditions of actual machining processes, MD simulations offer a reliable framework for understanding the influence of various factors on the material removal process, particularly in relation to the interaction between the tool and the workpiece.

Advancements in MD simulations have also facilitated a deeper understanding of the sub-surface changes that occur in silicon following indentation. This research has been pivotal in identifying the factors that contribute to surface integrity, an essential consideration in the machining of silicon. The ability of MD simulations to predict the outcomes of mechanical interactions at the nanoscale has also been validated by experimental practicees, emphasizing their predictive power. Consequently, the integration of MD simulations with experimental techniques has significantly contributed to enhancing the material removal strategies employed in the machining of silicon, leading to improvements in surface conditions, tool longevity, and overall machining efficiency.

1.3 Overview

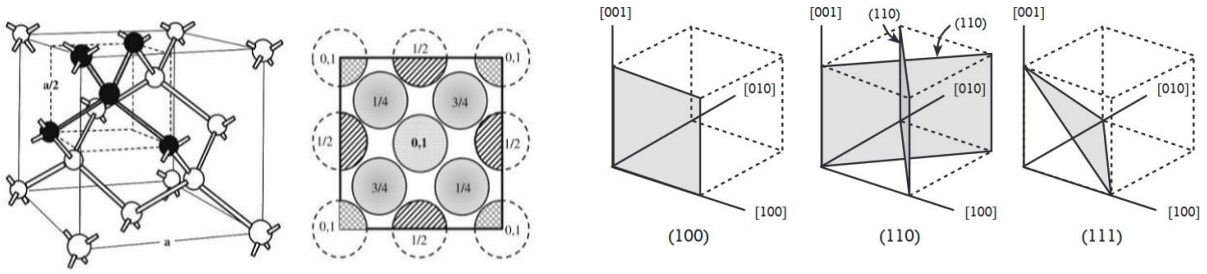
The objective in this thesis is to advance the comprehension of silicon's properties through molecular dynamics (MD) simulations. This computational method examines the movement of silicon particles within a system, enabling an analysis of their response to various manufacturing-relevant conditions such as applied forces and temporal changes. By enhancing the understanding of silicon's behavior through these simulations, it’s possible inform improvements in the manufacturing processes that involve this element, potentially leading to the optimization of products like electronic devices and solar panels. First, an overview of the important theoretical aspects is given, then the simulation setup and the data are described, as well as the results obtained and discussion for this and further research.

Literature review

This chapter is dedicated to the theoretical background concepts needed in this thesis and a literature review of the most recent scientific work done in this specific research area.

2.1 Monocrystalline silicon

Silicon (Si), the 14th element in the periodic table, is the second most common element in the earth's crust. It has a special crystal structure, known as the diamond cubic crystal structure, made up of 18 silicon atoms, as shown in Figure x. This silicon crystal is divided by several planes that cut through the atoms. These planes are labeled using a system called the Miller Indices. Mainly, there are three types of planes: (100), (110), and (111), as shown in Figure 2.1 [7]. In these conditions, a type of silicon called monocrystalline silicon is formed. This is a single crystal structure that doesn't have any breaks caused by grain boundaries [5].



(a) Crystalline structure *(b) Crystallographic planes*

Figure 2.1: *(a) Crystalline structure of silicon in the projections tree-dimensional and bi-dimensional [8] and (b) Crystallographic planes of monocrystalline silicon [9]*

Silicon as an anisotropic material, demonstrates properties that depend on its crystallographic orientation [6]. At room temperature, silicon is characterized by its brittleness and hardness, showing a significant tendency to fracture abruptly under tensile stress while exhibiting minimal plastic deformation [10]. The semiconducting nature of silicon makes it an ideal candidate for manufacturing solar panel wafers and electronic microchips [11]. However, the atomic configuration varies across different orientations of silicon. The susceptibility to fracture in the diamond cubic crystal structure is notably higher along a (110) surface compared to (100) or (111) surfaces [12]. Consequently, crystallographic orientations play a critical role in wafer production for specific applications.

Primarily, the (100) and (111) orientations, which are parallel to the unit cell face and intersect three opposite corners of the unit cell, are utilized for device fabrication. Conversely, substrates with a (110) plane are rarely employed due to their limited practical applicability [11,12]. The (100) orientation is particularly favored, being exclusively used in the production of CMOS (Complementary Metal-Oxide-Semiconductor) devices [12]. The presence of a rough wafer surface or residual damage can trigger premature cracking under stress. Consequently, polished wafers that adhere to the standards outlined by the Semiconductor Equipment and Materials International (SEMI) are preferred over damaged wafers, ensuring a mechanically defect-free surface [13].

2.2 Silicon wafers machining

Understanding the transition from ductile to brittle behavior is critical in wafer sawing machining processes. This shift in behavior is highly dependent on the specific conditions of the machining operation. Research indicates that under scenarios, such as when operating at lesser cutting depths, it's possible to machine silicon in a ductile mode [14].

As illustrated in Figure x, during the initial phases of cutting, silicon displays ductile properties. This leads to the creation of a smooth surface. However, as the depth of cut increases, a critical point, known as the critical depth of cut (dc), is reached where the first crack in the silicon material becomes evident. Once this critical depth is exceeded, the machining process transitions into a brittle phase. This phase of brittle machining is characterized by the emergence of small fractures and surface cracks on the silicon surface [11]. Therefore, the depth of the cut serves as a decisive factor in determining whether the machining operation will result in ductile or brittle behavior. [15, 16,17].

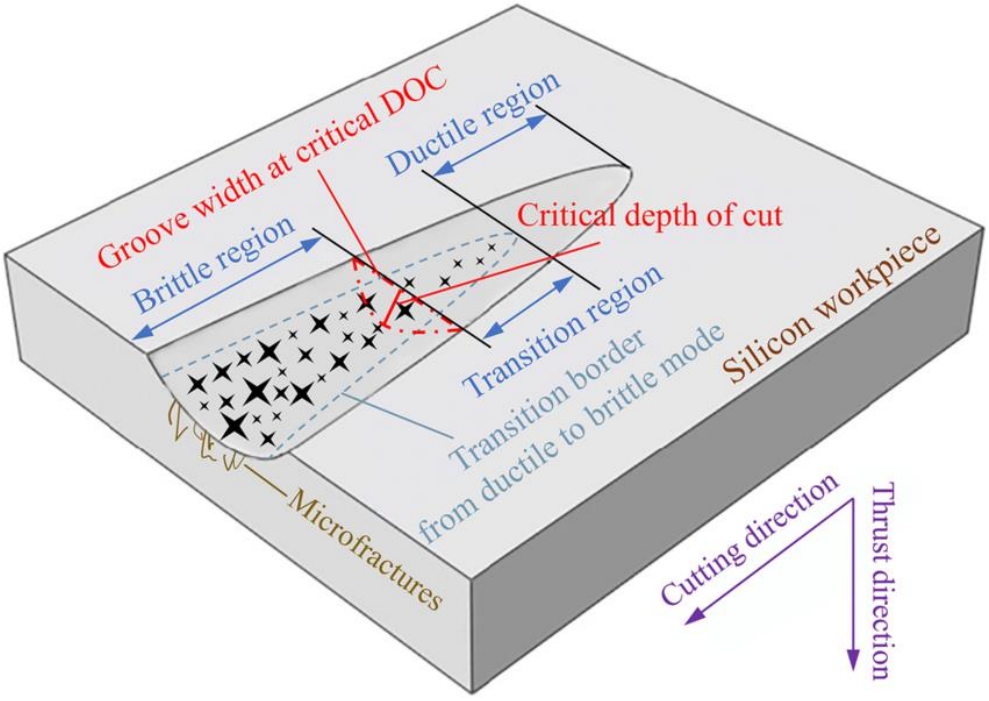


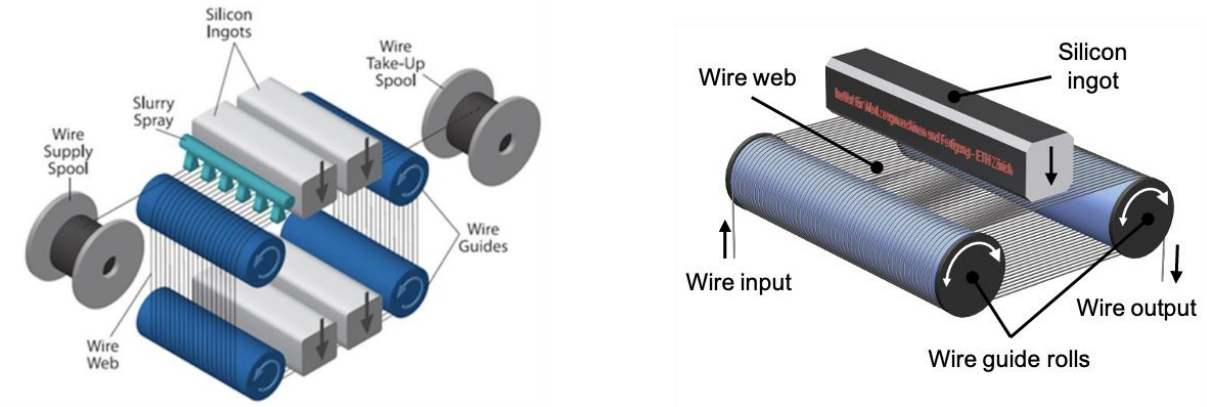
Figure 2.2: *Schematic of critical depth of cut identification. Extracted from [16]*

2.3 Loose abrasive and diamond wire sawing

In the field of silicon wafer sawing, two main process, Loose Abrasive Slurry Sawing (LAS) and Fixed Abrasive Sawing (DWS), have gained prominence, each distinguished by its unique material removal mechanisms and associated strengths and weaknesses. Loose Abrasive Slurry Sawing (LAS), a traditional method, uses a slurry comprised of abrasive silicon carbide (SiC) particles applied to a wire web . The process involves pressing silicon ingots against the wire web in an upward or downward direction until the desired cut is achieved. Material removal occurs due to the consistent interaction between the silicon surface and the SiC particles [5]. The primary mechanism identified in this process involves the creation of brittle fractures triggered by the rolling and indenting of grains. Despite being a well-established method, LAS is associated with slower cutting speeds and requires a substantial amount of wire and slurry [4,5].

Emerging as a newer technique, Fixed Abrasive Sawing leverages diamond-coated steel wires, referred to as diamond wire sawing (DWS), to execute the cuts. In this approach, the abrasive particles are affixed directly to the wire, thereby allowing the substitution of the traditional slurry with a water-based coolant. DWS has the advantage of facilitating significantly higher cutting speeds, requiring less wire, and relying only on an inexpensive cooling fluid such as water [4,10]. While the initial expenditure on diamond-coated wires may be higher, these wires are capable of removing a larger volumme of material by scratching the particles against the crystal surface. This material removal process is a combination of ductile and brittle removal, varying based on the penetration depth. Current theories propose that the pressure applied during the cutting process can induce phase transitions, thereby promoting ductile removal [5].

The Fixed Abrasive Sawing technique has received substantial adoption in the photovoltaic (PV) industry, where it is used in the production of about 90% of PV wafers. The evolution and contrast of these methodologies play a crucial role in understanding the progress and potential future trends in the silicon wafer sawing landscape. The two different processes (LAS and DWS) can be seen in Figure 2.3.



(a) *(b)*

Figure 2.3: *(a) Loose abrasive slurry sawing (extracted from [1] and (b) diamond wire sawing)*

Thus, the variation in sawing methodologies results in distinct mechanisms of material removal. The Load Assisted Sawing (LAS) method employs a mechanism that combines rolling and indenting actions of the grains, predominantly resulting in fracture-induced material removal, characterized by brittle fractures. In contrast, Diamond Wire Sawing (DWS) involves a grain that acts by scratching, which gives rise to a combination of ductile and brittle material removal, the proportion of which is contingent upon the depth of penetration [5]. It is posited that the pressure exerted during the sawing process induces phase transitions that facilitate ductile material removal.

2.4 Phase transitions

In the ductile-regime machining of silicon, which involves dislocation movements and crystal plastic deformation, the phenomenon of metallization is initiated due to the exertion of high-pressure beneath the cutting tool, consequently enabling phase transformations in silicon [18]. These transformations are triggered by the generation of immense hydrostatic stress, which goes beyond the pressure threshold necessary for new phase transitions. Under standard conditions, silicon maintains a cubic diamond structure, known as Si-I. This configuration remains stable until 11 GPa at room temperature and from absolute zero to its melting point at atmospheric pressure [19, 22]. However, when subjected to higher pressures, silicon can exhibit an additional 11 crystalline phases [20]. Most of these phases are exclusive to extremely high pressures, thus exceeding the relevance of this discussion. Certain phases achieve thermodynamic stability as pressure exceeds specific critical thresholds, emerging directly from the cubic phase [20, 21]. The crucial phases relevant to this context are S-II, Si-III, Si-IV, Si-IX, and Si-XII [20].

As shown in Figure 2.4 provides a diagram of the phase transformations that occur in silicon under static contact loading and subsequent annealing. Si-I is the single phase that is thermodynamically stable at ambient conditions. Rapid unloading rates (> 1 mm/min) suggest a lack of sufficient time for the silicon lattice to reform during pressure release, leading to lattice disorder and resulting in the formation of amorphous material, rather than the kinetically regulated Si-II to Si-XII phase change [19, 22].

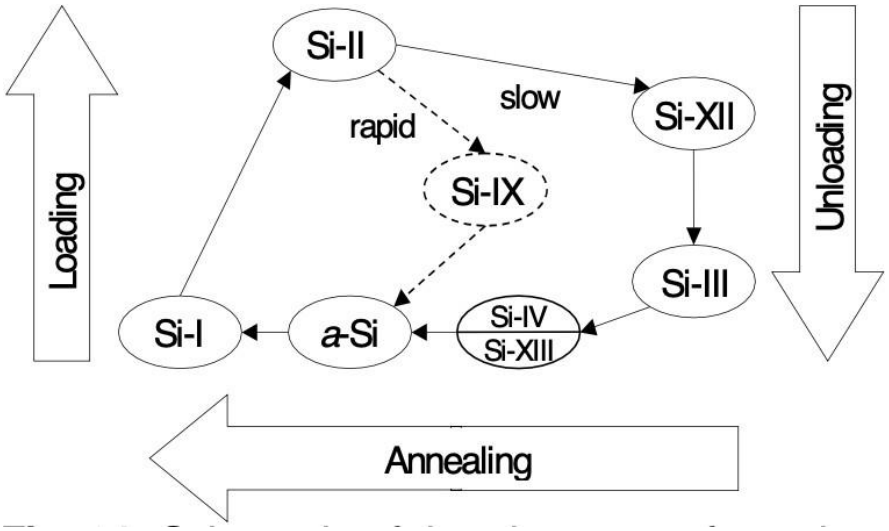


Figure 2.4: *Schematic of the phase transformations cycle in silicon under contact loading [20]*

Notation	Structure	Pressure region (GPa)
Si-I	Diamond cubic	0-12.5
Si-II	Body-centered tetragonal (*beta*-Sin)	8.8-16.0
Si-III	Body-centered tetragonal (basis of eight atoms)	2.1-0
Si-IV	Diamond hexagonal	-
Si-IX	Tetragonal (12 atoms per unit cell)	12-0.0
Si-XII	Trigonal (8 atoms per unit cell)	12-2.0

Table 2.4: *Crystalline phases of silicon and respective pressure region [21].*

An irreversible transition from Si-I to Si-II occurrs within a pressure range of 9 to 16 GPa [19,22]. The onset of irreversible plastic deformation in monocrystalline silicon only commences with the introduction of this metallic phase. Upon unloading, a change from a metallic tetragonal-body-centered phase to an amorphous phase is observed, as confirmed by studies involving electrical resistance, x-ray diffraction, Raman spectroscopy, and optical properties [22]. Upon pressure release, a transition from Si-II to other phases such as Si III, Si IV, Si-IX, and Si-XII is recognized. Si-XII forms first at pressures between 10 to 12 GPa, and with further pressure release, the level of rhombohedral distortion gradually decreases, yielding a mixture of Si-XII and Si-III (pressure release from 10 to 0 GPa). This transformation can be completely reversed by recompression to 2.5 GPa [20, 23].

In terms of the transformation to Si-IV, this phase can either originate from the metastable phase after heat treatment or from Si-I following plastic deformation. The transition from cubic to hexagonal phase is deemed martensitic, despite the hexagonal diamond structure in silicon not being a thermodynamically stable phase. This classification is due to its diffusionless mechanism and certain crystallographic

characteristics, such as the interface between the transformed and untransformed regions remaining nearly planar - a characteristic trait of martensitic transformation. The transformation sequence with increasing pressure is I → II → XI → V → VI → VII → X [19, 23, 24].

The individual phases exhibit distinct densities, and a volume alteration transpires during the phase transition. The sequence of densities discovered was ρSi-XII > ρSi-III > ρSi-I > ρSi-IV > ρa-Si [18]. The transformation from Si-I to Si-II is followed by a 20% material densification. Upon slow decompression, the transition from Si-II to Si-XII leads to a 9% volume expansion, with 2% recovery from the gradual Si-XII to Si-III transformation at low pressures, considering that the equilibrium Si-III structure was found to be 9% denser than Si-I and 2% less dense than Si-XII. Finally, the hexagonal diamond Si-IV phase has an atomic volume identical to that of Si-I. Owing to these density variations and residual stress, silicon wafers may warp during or after machining when the conditions fluctuate during the process or between thetwo faces, see Figure 2.5 which demonstrates scenarios that could result in the need for further post-processing of the wafer or, in some cases, lead to the wafer being deemed unsuitable.

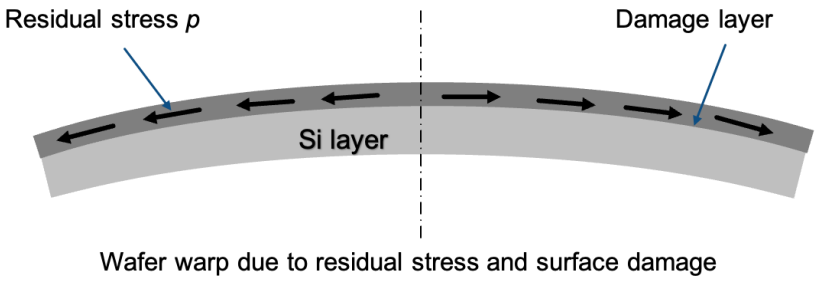


Figure 2.5: *Wafer warp due to residual stress and surface damage [26]*

2.5 Nanoindentation

Nanoindentation, a technique for measuring the mechanical properties of materials at the nanoscale, plays a role in understanding the behavior of materials under stress. This method involves the controlled application and removal of a load to a sample using a geometrically well-defined indenter as illustrated in Figure 2.6 where h_{max} is the maximum indentation depth and h_f is the displacement or depth at the beginning of the unloading process. The interaction between the indenter and the material produces a force vs. displacement curve, which serves as a detailed mechanical fingerprint of the material under test [27].

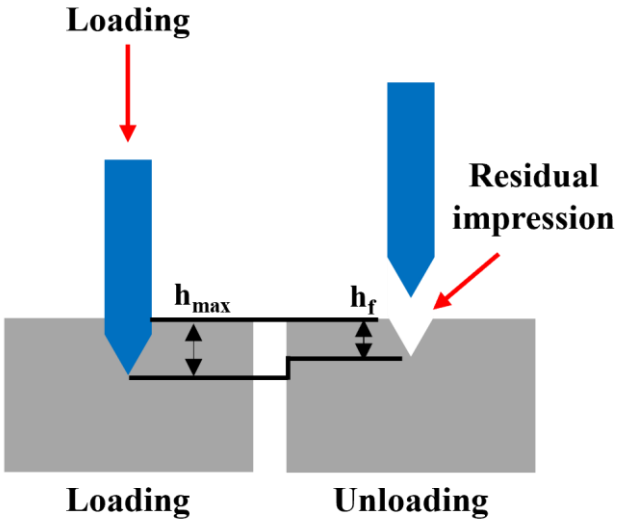


Figure 2.6: *Scheme showing the working principle of nanoindentation. Adapted from [44]*

One of the significant outcomes of nanoindentation tests on brittle materials, for example, silicon, is the observation of pressure-induced phase transformations. When loaded, the material directly the indenter transitions into a metallic state, which is ductile enough to allow for plastic deformation. Upon unloading, instead of reverting to its original state, silicon undergoes a transition into an amorphous structure or shifts into other metastable phases. This behavior is crucial for developing new machining techniques aimed at minimizing or eliminating the damage typically caused by traditional machining methods [28, 29].

Moreover, further research into the phase transformations occurring during nanoindentation has shown that these processes are influenced by several factors, including the shape of the indenter and the loading/unloading rates. These findings are crucial for selecting appropriate machining conditions, linking the shape of the indenter to the geometry of the machining tool, and the loading/unloading rates to the machining speed [28].

Furthermore, through the nanoindentation technique, it's possible quantitatively characterize the mechanical properties of small volumes of material, providing insights that are critical for the continued innovation and development of technologies also the insights gained from nanoindentation tests are invaluable for improving the mechanical, optical, and electronic properties of brittle materials. By understanding the deformation, fracture, and microstructural changes induced by indentation, researchers can devise strategies to minimize or eliminate machining damage, thereby significantly enhancing product performance [28, 29].

2.6 Molecular dynamics

Molecular Dynamics (MD) simulations have established as a potent tool for studying physical phenomena at the nanoscale, allowing for an in-depth investigation into the mechanical and tribological properties of materials. Through MD simulation, one can observe the behavior of atoms and molecules

under various conditions, providing deep insights into the underlying mechanisms governing material properties. This computational method, leveraging Newton's equations to simulate the motion of particles in atomic and molecular systems, has been applied across a wide range of fields, including material physics, chemistry, and biology, showcasing its versatility and ability to deliver valuable insights often inaccessible through traditional experimental methods [30]. In a conventional MD simulation, Newton's second law is used to update atomic positions in time

$$F_i = m_i a_i = -\frac{\partial U}{\partial r_i} \quad (2.1)$$

where F_i is the force on a particle i with a mass mi and an acceleration a_i, U is the interatomic potential energy and r_i represents the Cartesian set of coordinates of a particle i. The potential energy term (U) is described in section 4.3.

One area where MD has proven particularly useful is in understanding nanoindentation, an experimental method to measure mechanical properties such as hardness and elastic modulus at the nanoscale. For instance, Chen et al. (2008) utilized MD simulations to investigate nanoindentation on the (100) crystal surface of cyclotrimethylenetrinitramine (RDX), demonstrating the potential of MD simulations to reveal intricate details about substrate heating and subsequent molecular fragment release during nanoindentation [30, 31].

Furthermore, the nano-engineering of construction materials represents another promising application of MD simulations, as discussed by Lau et al. (2018). They highlight how understanding physical and chemical processes at the nanoscale is crucial for improving the macroscopic performance of construction materials such as concrete and cement. The potential of MD to provide insights into mechanical deformation and chemical reaction mechanisms in construction materials, paving the way for the development of new materials with enhanced properties through nano-engineering [31, 32].

Acord with Cui and Zhang (2017) discuss the fundamentals of nano-machining materials, including critical aspects such as the influence of tool geometry, material properties, and machining parameters on nano-indentation and nano-cutting processes. This study underscores the importance of MD simulation in identifying machining mechanisms and optimizing nanoscale manufacturing processes. The ability to simulate material behavior under extreme conditions and at atomic and molecular scales not only enhances the understanding of material science fundamentals but also enables the design and fabrication of systems with superior performance [22, 33].

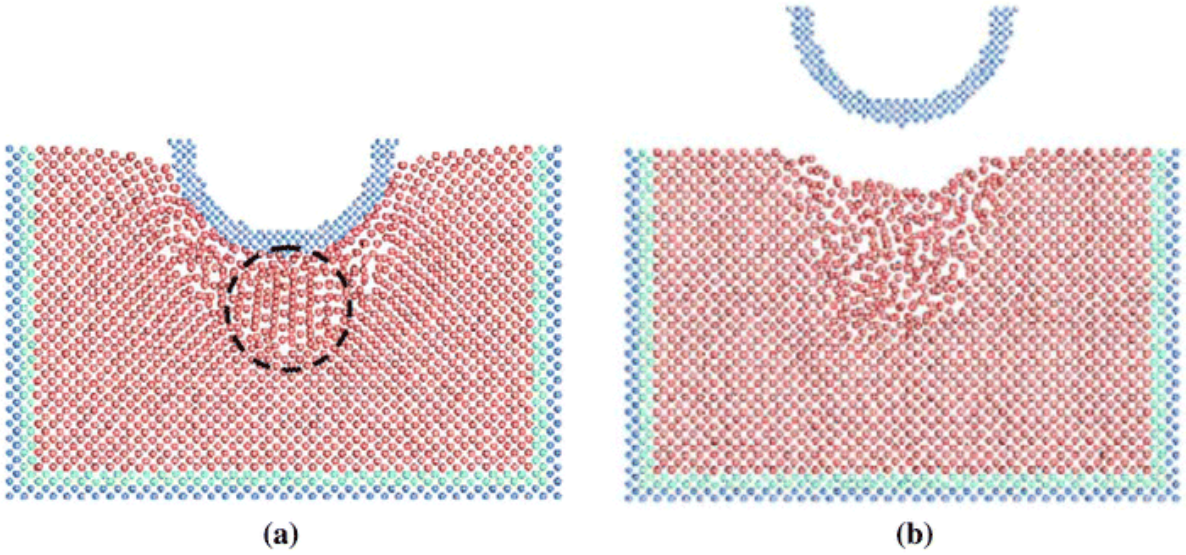


Figure 2.7: *Silicon phase transformation: a) Under maximum pressure from indentation, the atomic arrangement below the indentation tool is transformed, displaying a crystalline structure that deviates from the initially observed diamond cubic pattern, as indicated by the dashed enclosure; b) a shift from crystalline to amorphous structure is observed with the removal of the load. Extracted from [22].*

Together, these studies demonstrate the critical application and value of molecular dynamics simulations in modern material science research. By providing a window into processes at the atomic and molecular scale, MD allows for detailed exploration of material properties and deformation mechanisms, offering fundamental insights that can be used to improve manufacturing techniques and develop new materials with optimized properties for specific applications. As simulation techniques and computational power continue to evolve, the role of MD in material research is expected to expand further, opening new avenues for discoveries and innovations in nanotechnology and materials engineering.

2.7 Molecular dynamics and nanoindentation

The nanoindentation technique has become a foundation in the field of materials science for probing the mechanical properties of materials at the nanoscale. This method's efficacy is significantly enhanced by molecular dynamics (MD) simulations, which offer a microscopic view of material behavior under the stress of indentation. These simulations facilitate the application of an external force via a rigid indenter, leading to the plastic deformation of the material in question. The depth of indentation, alongside load-displacement curves and the stress and strain fields within the material, provides a rich dataset for analysis, allowing for a nuanced understanding of the deformation mechanisms and structural transformations that occur during the nanoindentation process [28].

A key factor in the fidelity of these simulations is the selection of appropriate interatomic potentials, which dictate the force and energy dynamics between atoms, thereby influencing the material's simulated mechanical behavior. The choice of boundary conditions is another crucial aspect, as it defines the simulation space and the constraints applied to the material, affecting the realism and applicability of the simulation results to real-world scenarios [30].

Combining experimental data with MD simulations paves the way for an atomistic-level exploration of material properties, offering insights into the effects of various boundary conditions and simulation parameters on material behavior. This integrative approach not only deepens on the understanding of the nanoindentation process but also aids in the design and optimization of materials with specific mechanical properties tailored to their intended applications [31].

In summary, MD simulations represent an invaluable tool in the study of nanoindentation, providing detailed atomic-level insights into material behavior and deformation mechanisms. The synergy between experimental techniques and computational simulations broadens thre comprehension of material properties, contributing to the advancement of materials science and engineering [28, 30].

2.8 LAMMPS

The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) has established itself as an indispensable tool in the realm of materials science for conducting classical molecular dynamics (MD) simulations across a wide spectrum of particle ensembles, including atoms, molecules, and larger entities within various states such as solids, liquids, and gases. Designed to accommodate a broad range of systems, from atomic to macroscopic scales, LAMMPS is proficient in simulations that utilize a diverse array of interatomic potentials and boundary conditions. Its capabilities span both two-dimensional (2D) and three-dimensional (3D) systems, adeptly handling simulations from a minimal number of particles to those encompassing billions of particles [39].

Optimized for parallel computing environments, LAMMPS efficiently operates across multicore servers, multi-CPU systems, distributed-memory clusters, and supercomputers. It harnesses the Message Passing Interface (MPI) for parallelization while integrating OpenMP multi-threading, vectorization, and GPU acceleration. The LAMMPS codebase, implemented in C++, is noted for its modularity and extensibility, enabling the easy integration of new force fields, atom types, and diagnostic tools, thereby broadening its applicability across various research domains. The efficiency of LAMMPS' in simulating nanoindentation on thin single-crystal FCC copper layers through peridynamics, highlighting its flexibility in applying both molecular dynamics and peridynamics within a unified framework [34, 36].

In the context of nanoindentation simulations, LAMMPS provides a comprehensive framework for examining the mechanical interactions of materials under indentation. This process entails setting up the initial atomic configuration, system stabilization through an equilibration phase, and the subsequent introduction of the indenter to apply forces or displacements. Yu, Liang, Chen, and Guo (2014) leveraged LAMMPS to study material deformation in monocrystal silicon during nanoindentation and nanocutting, offering insights into transformation laws and the impact of crystal orientation on machining. Similarly,

Chen et al. (2008) used LAMMPS to investigate the nanoindentation of RDX, noting significant heating and deformation effects, while Stewart and Spearot (2013) explored nanoindentation on the basal plane of crystalline MoS2, discussing mechanical responses, including local phase transformations beneath the indenter [36, 37].

Furthermore, LAMMPS' advanced modeling and simulation capabilities are exemplified in studies like those by Yu, Adams, and Hector (2002), who conducted high-speed nanoindentation simulations on Al substrates to examine various process variables and deformation mechanisms. Such research underscores LAMMPS' capacity to handle dynamic and complex simulations, reinforcing its central role in advancing materials science by facilitating the conceptualization and realization of novel materials with superior mechanical properties. Through its adaptability, comprehensive selection of potential fields, boundary conditions, and prowess in parallel computation, LAMMPS continues to propel the field of materials science forward, enabling detailed analysis and understanding of material behavior under nanoscale forces [34 - 38].

Research gap

While significant strides have been made in understanding silicon behavior, particularly in the context of silicon processing applications, there is a notable research gap in the molecular dynamics (MD) analysis of silicon atoms under diverse conditions. The existing body of literature provides valuable insights into the macroscopic properties of silicon-based materials, yet there is a lack of comprehensive investigation at the atomic scale using MD simulations.

Investigating the behavior of silicon atoms at the atomic level with molecular dynamics (MD) simulations is essential for understanding the complex processes involved in silicon manufacturing, improving its functionality, and learning how silicon atoms react to various types of molecular frame.

This identified gap in research emphasizes the importance of conducting structured studies on the atomic interactions within silicon through MD simulations. Such studies are particularly crucial for scenarios that directly impact silicon processing techniques.

Models and methods

This chapter is dedicated to the models and methods used. The simulation setup developed at the Institut für Werkzeugmaschinen und Fertigung (IWF), the simulation plan and procedure are described.

4.1 Silicon model

In this study configures a silicon (Si) atomic structure within a molecular dynamics (MD) framework, setting the lattice parameter in Angstroms to mirror the interatomic spacing in silicon's diamond cubic lattice structure. The simulation box, carefully dimensioned and a defined silicon block, with dimensions represented in Table 4.1, which becomes the central focus of the mechanical investigation. Each silicon atom is characterized by an atomic mass of 28.08 atomic mass units, a detail critical for the accuracy of dynamic simulations.

Parameter	**Description**
Lattice	5.43 Å
Simulation Box Dimensions	40 Å x 40 Å x 20 Å
Silicon Block Dimensions	20 Å x 20 Å x 10 Å
Atomic Mass of Silicon	28.08
Unit System	Metals
Time	Picoseconds
Modeling Style	Atomic
Boundary Conditions	Periodic
Crystal Structure	Diamond cubic

Table 4.1: *Parameters used in the silicon model.*

To ensure a realistic representation of atomic interactions, the study adopts the "metals" unit system common in computational materials science. The choice of an "atomic" modeling style is strategically made to balance computational efficiency with the need for precision. This approach enables the effective simulation of complex atomic behaviors within the silicon structure. Periodic boundary conditions are applied to the model to emulate an infinite lattice, a critical aspect that allows the simulation to reflect continuous material properties and behaviors. This setup is essential for capturing the long-range interactions characteristic of condensed-phase systems.

The selection of the diamond cubic lattice structure for the simulation foundation is a deliberate decision to match the intrinsic crystalline order of silicon, ensuring that the simulated behaviors and properties are

representative of actual silicon characteristics. This configuration sets the stage for an in-depth exploration of silicon's responses to mechanical forces and external perturbations at an atomic scale.

4.2 Indenter

In this simulation, the setup includes a silicon lattice and a Berkovich indenter, designed to closely resemble real-world conditions. The indenter, simulated of carbon atoms with the same atomic mass (12.011u), is used to test how the silicon lattice reacts when pressure is applied in a controlled way. Creating the indenter in the simulation involves a process that representing the properties and behavior of a real Berkovich indenter shape, a unique three-sided pyramidal shape (as shown in Figure 4.1)., which is commonly used in nanoindentation experiments to measure material properties. This choice ensures that the indenter not only replicates the physical properties of diamond but also its unparalleled hardness.

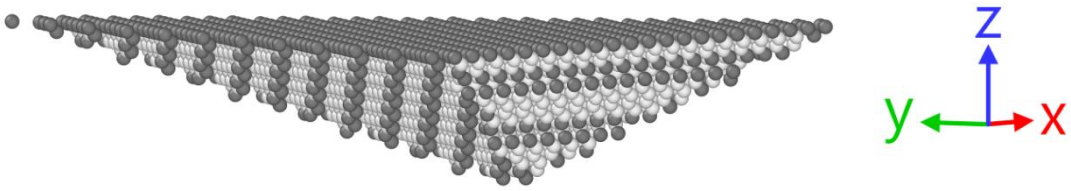


Figure 4.1: *Simulated Berkovich-type indenter [author].*

The creation process also involves setting the indenter's atomic mass and ensuring that the force it exerts is accurately modeled. The interactions between the carbon atoms of the indenter and the silicon atoms of the substrate are are simulated using mathematical models like the Tersoff potential, that will be seen in section 4.3. This model accurately calculates the forces and energies involved in the interactions between the indenter and the silicon, considering the repulsive and attractive forces that come into play at the atomic level. By meticulously modeling the indenter's composition, shape, and interaction with the silicon substrate, the simulation can closely emulate the mechanical response of silicon under controlled conditions.

4.3 Tersoff potential

The Tersoff potential introduces an approach to calculating the energy between two atoms. It combines terms that represent both repulsive and attractive forces, with the attraction modulated by the bond order. This bond order is a dynamic quantity that changes based on the number and arrangement of neighboring atoms, reflecting how in a dense atomic environment, an atom will form weaker bonds due to the shared

distribution of bonding electrons.

The general equation for the Tersoff potential is:

$$E_{ij} = A_{ij}\ \exp\left(-\lambda_{ij} r_{ij}\right) -\ B_{ij} \exp\left(-\mu_{ij} r_{ij}\right) \quad (4.1)$$

where A_{ij} and B_{ij} denote the repulsive and attractive potentials, respectively, and λ_{ij} signifies the bond order between atoms *i* and j, inversely proportional to bond coordination.

In the computational investigation of silicon's atomic interactions, the Tersoff potential is employed as a model designed to capture the nuanced dynamics of bond strength variation within the material's structure. This potential diverges from conventional computational methods by accounting for the influence of the local atomic environment on bond formation and strength. Recognizing that atoms within a densely populated neighborhood form weaker bonds—a phenomenon crucial for accurately simulating material behaviors at the atomic scale—the Tersoff potential enables the detailed prediction and manipulation of silicon's material properties. It has thus become an indispensable tool in the materials science and engineering domain, facilitating profound insights into the behaviors and properties of silicon and other materials with similar bonding characteristics.

Silicon presents unique computational challenges due to its diamond cubic structure and the directional nature of its covalent bonds. Traditional computational models, which base interaction energies solely on atomic distances, fall short of capturing the complex interplay of forces within silicon. The Tersoff potential, however, dynamically adjusts the bond strength in response to the local atomic environment, employing a formula that integrates both repulsive and attractive forces along with the distance between atoms. This approach provides a more accurate representation of silicon's atomic interactions, reflecting the variability of bond strength in environments with high atomic density and making it particularly suitable for silicon simulations.

The foundational equation of the Tersoff potential, specifying the energy interactions between atoms, underpins the forthcoming discussions. What follows is an elucidation of a cutoff function to model the waning impacts of atomic interactions and the methodology for bond order calculation considering the proximity of neighboring atoms. These elements are crucial for the precise modeling of materials' behavior, particularly silicon, and pave the way for understanding the environmental dependence that enhances the simulation of complex material systems:

Cutoff Function: A cutoff function, $f_c(r_{ij})$ ensures that the effects of potential energy decline smoothly beyond a specific interatomic threshold, thus mirroring the finite influence range characteristic of atomic forces in materials like silicon.

Bond Order Calculation: The bond order, $\lambda_{ij} = (1 + \beta^n \zeta_{ijn})^{-\frac{1}{2n}}$, is computed to reflect the influences of neighboring atoms and their spatial configurations, a critical aspect for accurately modeling the directional covalent bonds inherent in silicon's structure. Where it adjusts the bond strength (λ_{ij}) based on the local atomic environment—specifically, the impact of neighboring atoms and their spatial configuration (ζi_{jn}), with β and n modulating this relationship.

Integral to the process of optimizing the Tersoff potential for simulations involving silicon is a detailed refinement of the model's parameters and the strategic implementation of specific functions. Key to adapting the Tersoff potential for silicon simulations are:

$$V_{ij} = f_c(r_{ij}) \left[A_{ij} \exp\left(-\lambda_{ij} r_{ij}\right) - B_{ij} \exp\left(-\mu_{ij} r_{ij}\right)\right] \quad (4.2)$$

In the potential for silicon, V_{ij} represents the interaction energy between atoms i and j, adjusted by the cutoff function $f_c(r_{ij})$ .This function ensures interactions beyond a certain distance don't contribute to the energy, enhancing realism and efficiency, A_{ij} and B_{ij} are coefficients for repulsive and attractive forces, respectively. $\exp\left(-\lambda_{ij} r_{ij}\right)$ and $\exp\left(-\mu_{ij} r_{ij}\right)$ reflect how these forces diminish with distance, where λ_{ij} and μ_{ij} modify the decay rate, essential for modeling silicon's behavior.

The choice of the Tersoff potenial for silicon simulations is predicated on its capacity to dynamically modulate bond strengths according to the local atomic environment, thus enabling a detailed and accurate depiction of silicon's material properties. This modeling capability is indispensable for elucidating silicon's behavior under a variety of conditions, which is crucial for the advancement of technologies in semiconductors, photovoltaics, and nanotechnology. By providing a granular understanding of silicon at the nanoscale, the Tersoff potential enhances the design and optimization of silicon-based materials and devices.

4.4 Parameters simulation

In a molecular dynamics (MD) simulation, each parameter plays a critical role in defining the scope and resolution of the study. The timestep, dictates the granularity with which the simulation captures the motion of atoms. A smaller timestep means the simulation can more precisely track the changes in the system, crucial for observing the dynamics of silicon's response to external forces on an atomic scale as shown in Table 4.1.

Parameters	Values
Timestep (ps)	0.1
Speed (Å /ps):	0.005
Thermo (steps):	100
Thermo (steps)	40.000

Table 4.2: *Parameters used in the simulation.*

The speed parameter refers to the rate at which a simulated process, such as the movement of an indenter, occurs. It is a key factor in rate-dependent studies, affecting how the material responds to external perturbations over time. The thermo steps are intervals at which the simulation outputs thermodynamic information. This regular reporting is vital for tracking the system's state and ensuring that the simulation remains on course, reflecting expected physical behaviors and conditions. Run steps define the total number of iterations the simulation will perform, thus setting the overall duration of the MD simulation, this duration is integral for observing the full spectrum of the material's response.

Results and Discussion

This section is dedicated to summarizing the results of the simulation.

5.1 Simulation results

5.1.1 Phase transition

As shown in Figure 5.1 it highlights the primary arrangement of silicon atoms into a diamond cubic lattice, characterized by each atom being connected to two others, thereby presenting a coordination number of 2. This specific structural form contrasts sharply with the face-centered cubic (FCC) phase, in which silicon atoms are each surrounded by six neighbors, resulting in a coordination number of 6. This contrast forms the basis of the exploration into how these distinct atomic arrangements influence the physical properties and responses of silicon.

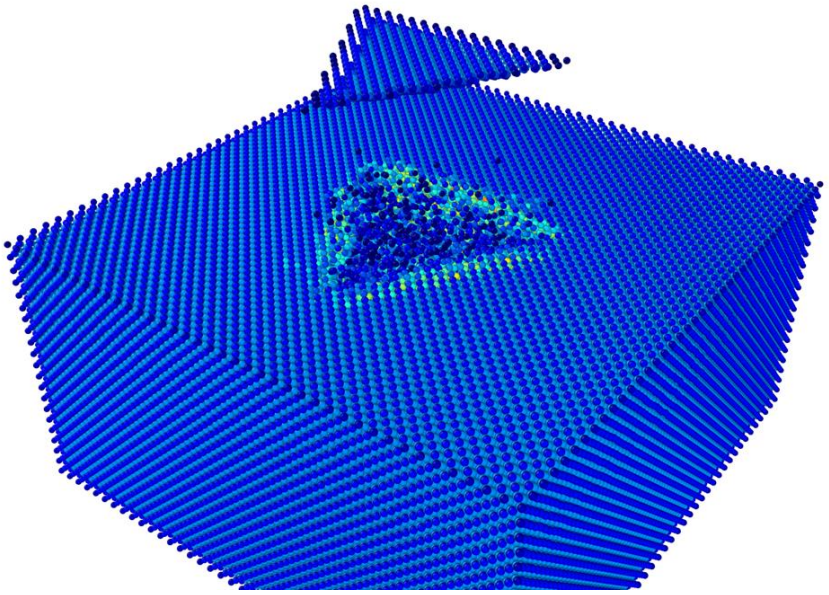
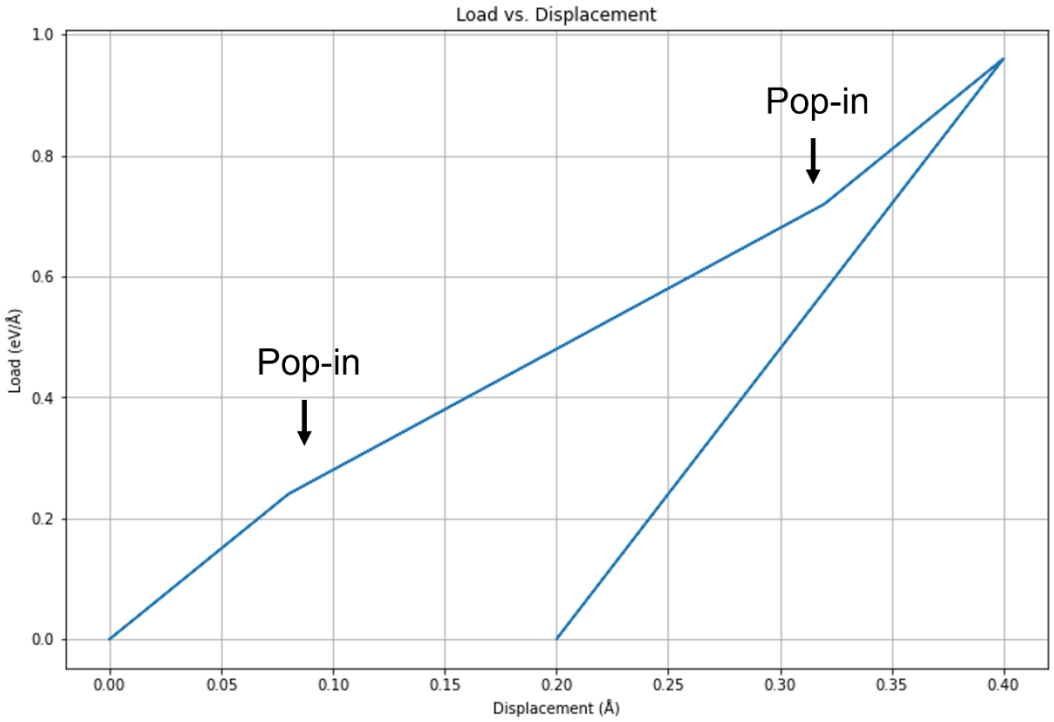


Figure 5.1: *Visualization a simulated Berkovich-type indenter interacting with a silicon substrate. The indenter's penetration into the substrate illustrates the local deformation and phase transformations at the atomic level.*

Applying the displacement vectors modifier from OVITO (visualization software), the study quantified the displacement vectors by comparing the initial positions of particles in a reference frame to their subsequent positions. This analysis rendered both a visual representation and a scalar quantification of each particle's movement, encapsulating the atomic-scale dynamics of the material under study. Figure 5.1 offers a compelling visualization of the silicon structure undergoing an indentation process. The visible deformation induced by the indenter, characterized by a notable change in the atomic arrangement. The variation in color among the atoms suggests alterations in potential energy and coordination, hinting

at dislocation events or phase transitions.

In the mechanical response under applied stress, initially, the relationship between load and displacement is linear see Graph 5.1, a characteristic feature of elastic deformation where the silicon lattice is temporarily distorted. Within this regime, the interatomic forces intrinsic to the monocrystalline structure can return the lattice to its initial state post-deformation.



Graph 5.1: *Load versus displacement curve from a nanoindentation experiment on a crystalline material, showing two 'pop-in' events.*

In the loading curve, when a line runs parallel to the displacement axis, it often signals a phase change, a discontinuity, or both. This phenomenon is referred to as a "pop-in." Conversely, when a similar event is observed during the unloading phase, it is termed a "pop-out." Unlike pop-ins, pop-outs invariably suggest that a phase transformation has occurred. The P-h curve (load versus displacement curve) depicted in Figure 4 illustrates two instances of pop-ins, with no evident pop-out events. The initial pop-ins are brief and occur prior to the emergence of the first dislocation, while the subsequent ones arise amidst the presence of dislocations, marking the plastic regime. During these instances, the potential for new phase formation beneath the indenter's tip is hindered by dislocationns.

Most notably, at higher displacement levels, a tendency to revert to a linear pattern. This intriguing phenomenon suggests that the monocrystalline silicon may be undergoing a phase transformation due to the applied load. Such a transformation is theorized to result in a structural rearrangement of the silicon atoms from the standard diamond cubic structure to a denser metallic phase. The incremental nature of this transformation could be indicative of a complex interplay between the nucleation of the new phase and the integrity of the original lattice, potentially facilitated by the pristine quality of the monocrystalline silicon used in the simulation.

5.1.2 Displacement

This section presents a "Displacement vs. Time" plot, illustrating the dynamic behavior of silicon when subjected to an external force over time, with measurements taken in picoseconds, Graph 5.2 reveals the displacement in angstroms, shedding light on the intricate atomic movements within the silicon lattice and how these atoms adjust under mechanical stress.

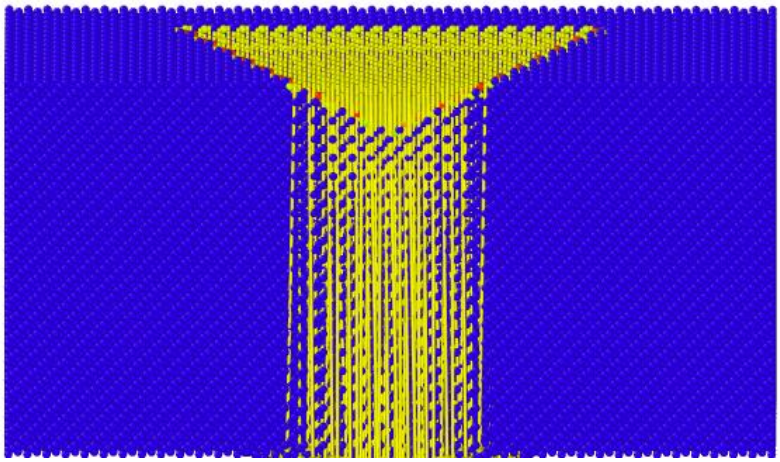
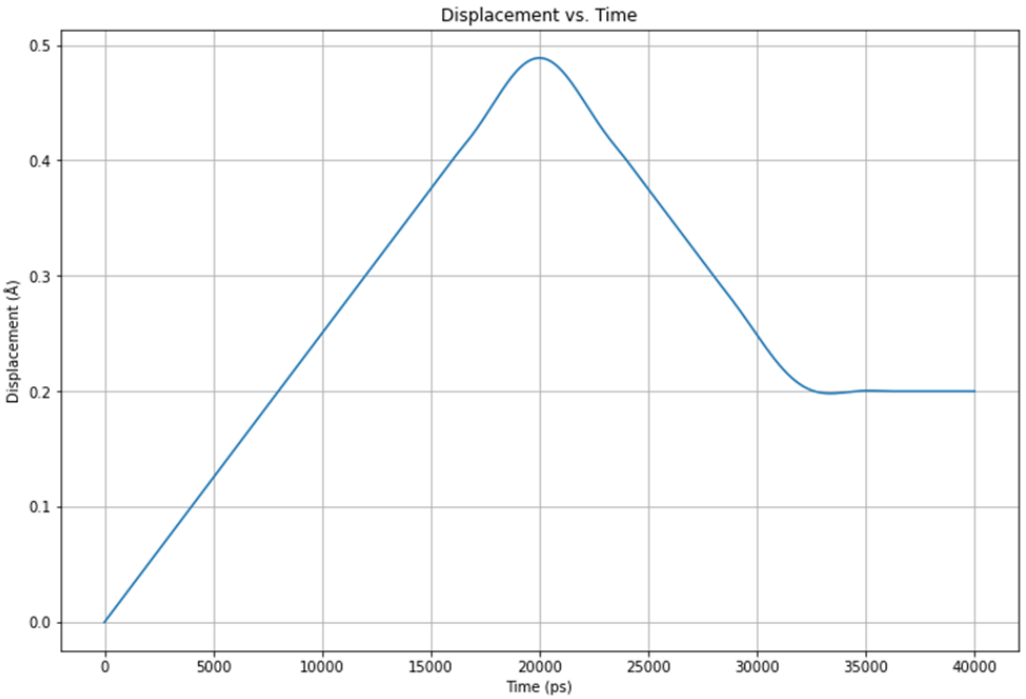


Figure 5.2: Cross-sectional view of a simulation highlighting the vectors direction in the material after the indentation.

In Figure 5.2, the aftermath of indentation is depicted through yellow vectors that extend from the indenter at the peak of the image, mapping out the displacement fields across the silicon. These vectors highlight the direction and scale of atomic displacements triggered by the indentation force. A notable deformation zone emerges beneath the indenter, where atoms are significantly displaced downward, pointing to a substantial disruption in the lattice structure. The vectors' symmetrical spread around the indentation site mirrors the crystalline silicon's isotropic properties, displaying a consistent deformation pattern under the exerted stress. This symmetry, along with the vectors' density, signals a focused stress concentration, potentially causing plastic deformation in the material.



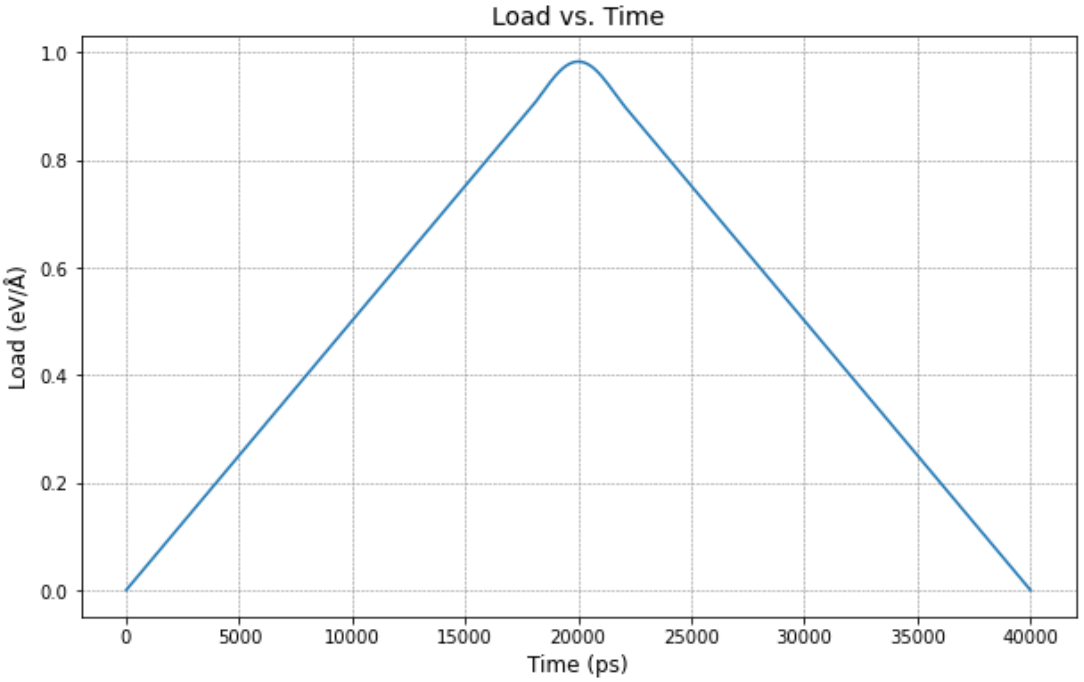
Graph 5.2: *A plot showing displacement (in angstroms) as a function of time (in picoseconds) during a simulated indentation process.*

The initial segment of the graph, showing a linear rise in displacement up to approximately 20,000 picoseconds, indicates that the silicon atoms are being uniformly influenced by a consistent force, moving at a steady rate. This portion of the curve suggests elastic deformation of the material, where the displacement is in direct proportion to the force applied.

After reaching peak displacement, a marked decline is observed, indicating a decrease in the applied force and a consequent contraction of the silicon structure. Nonetheless, the displacement does not revert to zero, implying that the material has sustained some irreversible deformation or has settled into a new equilibrium state. The asymmetry in the curve's descending section points to the fact that silicon's deformation encompasses more than just elastic behavior, including potential plastic deformation or a change in phase. The enduring displacement at the end of the time series reveals that the silicon has undergone a transformation affecting its atomic configuration, possibly leading to defect formation or a phase shift.

5.1.3 Load

The response of silicon to mechanical load is quantitatively is shown in the Graph 5.3. The dynamics essential for investigating the mechanical properties of silicon at the atomic scale. The load, expressed in electron volts per angstrom, serves as a measure of the force exerted per unit length within the material.



Graph 5.3: *Load-time graph from the simulation showing the progressive application and subsequent removal of force (measured in eV/Å) over time (in picoseconds).*

Upon analysis, culminating at a peak value of 1 eV/Å at approximately 20,000 picoseconds, indicative of the maximum stress applied to the silicon substrate. Subsequently, the load follows a linear decrease back to the initial state, mirroring the ascent in its progression. The symmetry observed in the load application and its subsequent release suggests an elastic deformation of silicon, with no discernible hysteresis effect within the time frame of the simulation. The maximum load-bearing capacity of silicon, as demonstrated by the peak stress level, provides a crucial metric for the elastic limits of the material.

5.1.4 Shear strain

The shear strain results are presented through a color-coded strain map (see Figure 5.3), illustrating the variation in shear strain throughout the silicon lattice as a result of the indentation processs.

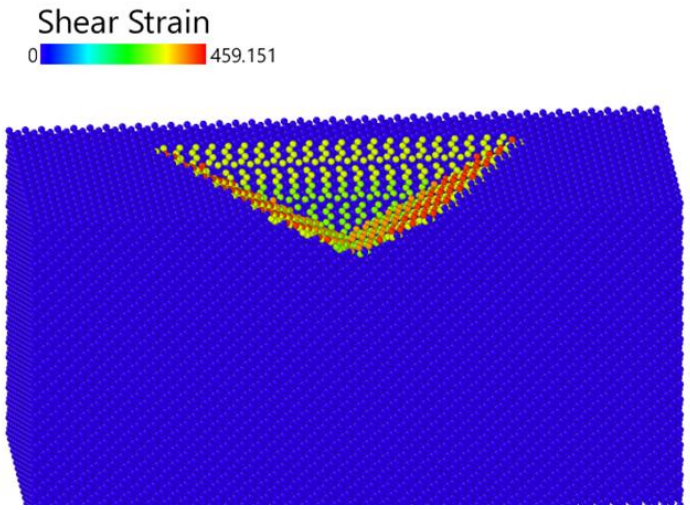


Figure 5.3: *Distribution of shear strain in the silicon substrate during the indentation simulation.*

The structure is marked by a gradation in color from blue at the edges to red at the center, indicating a range of shear strain levels. The area depicted in red, found at the indentation site's periphery, highlights the zone of highest strain where stress concentration peaks due to the force exerted by the indenter. The gradual shift in color from red to blue, moving away from the point of indentation, reflects a diminishing intensity of shear strain.

5.1.5 Particle identifier

The color-coding system, referred to as 'Particle Identifier' shown in Figure 5.4, distinguishes individual silicon atoms by their levels of displacement resulting from the indentation force.

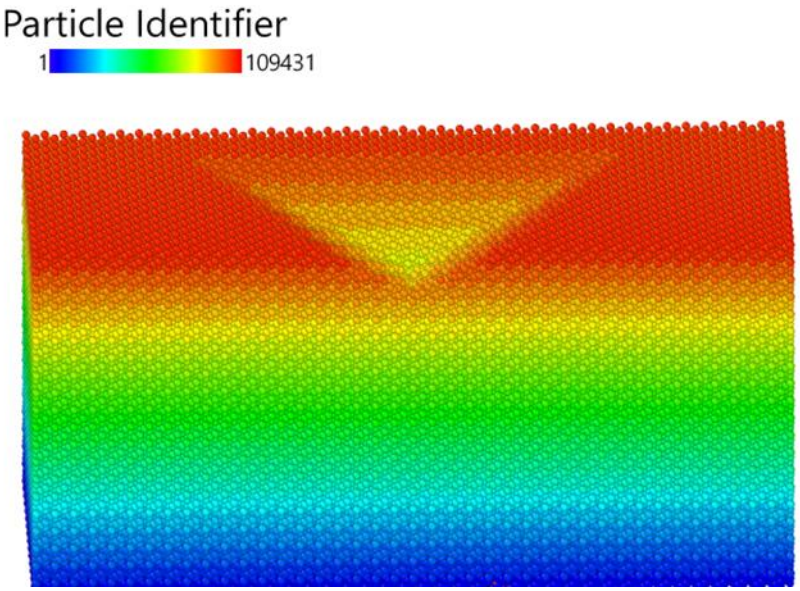


Figure 5.4: *A particle identification scheme. The multitude of particles is categorized by a unique identifier, with the color gradient from blue to red indicating the sequential tagging of particles.*

As shown in Figure 5.4, the color gradient ranging from blue to green, then yellow, and ultimately red, signifies increasingly severe atomic displacements. The apex of the indentation, marked in red, indicates the area of highest stress and greatest atomic disruption, pointing to where the lattice is most dramatically altered. This central zone is most susceptible to defects or phase changes, owing to the intense stress concentration present. Around this central peak, the color transition to yellow and green highlights regions under lesser strain, illustrating the dissipation of stress through the monocrystalline lattice. These varying colors represent the material's mechanical reactions to the applied load, visually mapping out the stress distribution and the deformation gradient within the silicon.

Conclusion and Future Work

6.1 Conclusion

Simulations were carried out to explore the behavior of silicon atoms during nanoindentation tests, a subject that has received limited attention in detailed studies. The research employed a Berkovich indenter in the simulations to conduct the investigation. On average, each simulation round required approximately seven hours of processing time. Data including stress, strain, and the positions of atoms over time were collected using the LAMMPs software commands and were visualized with the help of OVITO, a visualization software. The analysis concluded that:

1 Dynamic Behavior of Silicon: The "Displacement vs. Time" plot reveals the silicon atoms adjustments to mechanical stress over time, indicating a transition from elastic to potentially plastic deformation or phase change, as suggested by the irreversible displacement observed after the application of force.

2 Phase Transition: The displacement vectors and analysis of load versus displacement curves, reveals the elastic to plastic deformation transition, characterized by "pop-in" events, and hints at phase transformations under higher loads.

3 Mechanical Load: Silicon's capacity to undergo elastic deformation up to a certain stress level (1 eV/Å), with the subsequent release of load suggesting a reversible, elastic response within the simulation timeframe.

4 Particle Identification System: The 'Particle Identifier' system, using a color gradient to represent different levels of atomic displacement, serves as an effective tool in mapping out stress distribution and deformation gradients, identifying areas of highest stress and potential for defects or phase changes.

In summation, the employment of molecular dynamics simulations in this study has shown the exploration of material behaviors but has also provided a path for analysis. The findings shown the potential of this method for future research, paving the way for breakthroughs in understanding materials at the most fundamental level.

6.2 Future Work

In this thesis, a method to simulate the behavior of the silicon behavior under a pressure was presented. Considering that, the material can show different phases within different conditions, it is important to conduct further investigation on where this comes from.

In future research stands to gain from broadening the scope to include a variety of materials. This expansion would deepen the understanding of how different materials act and respond under varied conditions, enhancing knowledge beyond currently studied substances. Adjusting and fine-tuning simulation settings is also crucial. Modifying parameters like temperature and pressure can make simulations more reflective of real-life situations and increase the accuracy of their outcomes.

Exploring how the size of a material can influence its properties presents an intriguing direction for investigation. Examining materials at both microscopic and larger scales could reveal whether the principles observed at one scale are applicable at another. Comparing simulation findings with experimental data is another valuable step. This comparison can confirm the reliability of simulation methods and bolster confidence in their predictions of material behavior.

In conclusion, by examining a wider array of materials, refining simulation methods, investigating size effects, and cross-referencing findings with actual experiments, a more comprehensive understanding of materials can be achieved, which in turn can refine the application of simulations in materials science.

Bibliography

[1] A. Kumar and S.N. Melkote. “Diamond Wire Sawing of Solar Silicon Wafers: A Sustainable Manufacturing Alternative to Loose Abrasive Slurry Sawing”. In: Procedia Manufacturing 21 (2018). 15th Global Conference on Sustainable Manufacturing, pp. 549–566.

[2] Global market outlook, ed. Report of European photovoltaic industry association. 2012.

[3] Navigant Research, ed. Report Navigant Consulting Solar PV market forecast; 2012.

[4] H-J. Möller. Chapter 18 - Wafer processing. Ed. by P. Rudolph. Elsevier, 2015.

[5] “Chapter 12.- Wafer cleaning, etching and texturization”. In: Handbook of Photovoltaic Silicon.Ed. by D. Yang. Springer, 2019.

[6] W.C O’Mara, R.B Herring, and L.P Hunt. INSPEC, 2009.

[7] A. Bidiville. “Wafer sawing processes: from microscopic phenomena to macroscopic properties”.PhD thesis. 2010.

[8] B. El-Kareh and L.N Hutter. Silicon Analog Components. 2015.

[9] N. Maluf. An Introduction to Microelectromechanical Systems Engineering. Artech House, Inc, 2002.

[10] M. Tilli. “Chapter 4 - Silicon Wafers: Preparation and Properties”. In: Handbook of Silicon Based MEMS Materials and Technologies (Second Edition). Ed. by M. Tilli et al. Second Edition. Microand Nano Technologies. Boston: William Andrew Publishing, 2015, pp. 86–103.

[11] R. Hull, ed. Properties of crystalline silicon. 1999.

[12] D.R Evans. Crystal structure and growth - Microelectronic Device Fabrication 1. Lecture notes. Portland State University - USA, 2014.

[13] M. Tilli and A. Haapalinna. “Chapter 1 - Properties of Silicon”. In: Handbook of Silicon Based MEMS Materials and Technologies (Second Edition). Ed. by M. Tilli et al. Second Edition. Microand Nano Technologies. Boston: William Andrew Publishing, 2015, pp. 3–17.

[14] P.A.N Bernardini. Análise de Falhas em materiais vol 1. Lecture notes. Universidade Federal deSanta Catarina, 2020.

[15] G. Bifano, A. Dow, and O. Scattergood. “Ductile-regime grinding of brittle materials: Experimental results and the development of a model”. In: Advances in Fabrication and Metrology for Optics and Large Optics (1989).

[16] He, Wenbin & Liu, Changlin & Xu, Guoqing & Zhang, Jianguo & Xiao, Junfeng & Chen, Xiao & xu, Jianfeng. (2021). “Effect of temperature on ductile-to-brittle transition in diamond cutting of silicon”. The International Journal of Advanced Manufacturing Technology. 116. 1-16. 10.1007/s00170-021-07701-3.

[17] W. Huang et al. “A predictive model of critical depth of cut for ultrasonic elliptical vibration cutting of brittle materials”. In: 9th International Symposium on Advanced Optical Manufacturingand Testing Technologies: Advanced Optical Manufacturing Technologies. Ed. by Xiong Li et al.Vol. 10838. International Society for Optics and Photonics. SPIE, 2019, pp. 82–91.

[18] K. Afa and P. Capper. Springer US, 2013.

[19] T. Juliano, V. Domnich, and Y. Gogotsi. “Phase transformations under dynamic loading”. In: High-Pressure Surface Science and Engineering. 2004, p. 20. ISBN: 9780429144097.

[20] P. Pirouz et al. “The martensitic transformation in silicon—I experimental observations”. In: Acta Metallurgica et Materialia 38.2 (1990), pp. 313–322.

[21] V. Domnich and Y Gogotsi. “Phase Transformations in Silicon Under Contact Loading”. In: Rev. Adv. Mater. Sci. 3 (Jan. 2002).

[22] M. Ganchenkova and R.M Nieminen. “Chapter 9 - Mechanical Properties of Silicon Microstructures”. In: Handbook of Silicon Based MEMS Materials and Technologies (Second

Edition). Ed. by Markku Tilli et al. Second Edition. Micro and Nano Technologies. William Andrew Publishing, 2015, pp. 253–293.

[23] L.C. Zhang and W.C.D. Cheong. “Molecular dynamics simulation of phase transformations in monocrystalline silicon”. In: High-Pressure Surface Science and Engineering. 2004, p. 63. ISBN:9780429144097.

[24] Pirouz. P. et al. “The martensitic transformation in silicon—III. comparison with other work”. In: Acta Metallurgica et Materialia 38.2 (1990), pp. 329–336.

[25] U. Dahmen et al. “The martensitic transformation in silicon—II. crystallographic analysis”. In: Acta Metallurgica et Materialia 38.2 (1990), pp. 323–329.

[26] J.F. Cannon. “Behavior of the Elements at High Pressures”. In: Journal of Physical and Chemical Reference Data 3 (1974).

[27] S. Gao et al. “Warping of silicon wafers subjected to back-grinding process”. In: Precision Engineering 40 (2015), pp. 87–93.

[28] Sato, Y., Shinzato, S., Ohmura, T. et al. “Unique universal scaling in nanoindentation pop-ins”. Nat Commun 11, 4177 (2020)

[29] Wang S, Liu H, Xu L, Du X, Zhao D, Zhu B, Yu M, Zhao H. “Investigations of Phase Transformation in Monocrystalline Silicon at Low Temperatures via Nanoindentation”. Sci Rep. 2017 Aug 17;7(1):8682.

[30] Domnich, Vladislav & Gogotsi, Yury. “Phase Transformations in Silicon Under Contact Loading”. Rev. Adv. Mater. Sci.. 3. (2002).

[31] Daan Frenkel and Berend Smit. “Understanding Molecular Simulation”. Academic Press, Inc. 6277 Sea Harbor Drive Orlando, FL, United States (2001.).

[32] Chen, Y.-C., Nomura, K., Kalia, R. K., Nakano, A., & Vashishta, P. “Molecular dynamics nanoindentation simulation of an energetic material”. Applied Physics Letters, 93, 171908 (2008).

[33] Lau, D., Jian, W., Yu, Z., & Hui, D. (2018). “Nano-engineering of construction materials using molecular dynamics simulations: Prospects and challenges”. Composites Part B: Engineering (2018).

[34] Kim D, Oh S “Atomistic simulation of structural phase transformations in monocrystalline silicon induced by nanoindentation”. Nanotechnology 17:2259 (2006).

[35] Cui, D., & Zhang, L. “Nano-machining of materials: understanding the process through molecular dynamics simulation”. Advances in Manufacturing, 5, pp. 20-34 (2017).

[36] Ahadi, A., Hansson, P., & Melin, S. “Indentation of thin copper film using molecular dynamics and peridynamics”. Procedia Structural Integrity, 2, pp 1343-1350 (2016).

[37] Yu, N., Liang, Y., Chen, J. X., & Guo, Y. (2014). “Simulation Study of Material Deformation in Monocrystal Silicon Nano-Machining”. Key Engineering Materials, 621, 32-37. (2014).

[38] Chen, Y.-C., Nomura, K., Kalia, R., Nakano, A., & Vashishta, P. “Molecular dynamics nanoindentation simulation of an energetic material”. Applied Physics Letters, 93, 171908 (2008).

[39] Stewart, J. A., & Spearot, D. “Atomistic simulations of nanoindentation on the basal plane of crystalline molybdenum disulfide (MoS2)”. Modelling and Simulation in Materials Science and Engineering, 21 (2013).

[40] Yu, H., Adams, J. B., & Hector, L. G.“Molecular dynamics simulation of high-speed nanoindentation. Modelling and Simulation in Materials Science and Engineering, 10, 319-329 (2002).

[41] "LAMMPS Molecular Dynamics Simulator." Sandia National Laboratories, 2023, https://www.lammps.org.

[42] Tersoff, J. "New empirical approach for the structure and energy of covalent systems." Physical

Review B 37, no. 12 (1988): 6991.

[43] Maroudas, Dimitrios, and Lincoln J. Lauhon. "Mechanical properties of nanoscale materials." In Nanotechnology, edited by George Timp. Springer, New York, NY, 1999.

[44] Dahal, Tulashi & Gahlawat, Sonika & Jie, Qing & Dahal, Keshab & Lan, Yucheng & White, Ken & Ren, Zhifeng. (2015). “Thermoelectric and mechanical properties on misch metal filled p-type skutterudites Mm0.9Fe4−xCoxSb12 Thermoelectric and mechanical properties on misch metal filled p-type skutterudites Mm 0.9 Fe 42x Co x Sb” 12. 117. 55101-63722.