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# Molecular Dynamics (MD) Applications in Materials Science and Engineering and Nanotechnology

**Rishaad Khan**

North Brunswick Township High School, North Brunswick, US
Email: radishranger123@gmail.com

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## Abstract

Molecular dynamics (MD) is a computer simulation technique that helps to explore the behavior and properties of molecules and atoms. MD has been used in research and development in many spaces, including materials science and engineering and nanotechnology. MD has been proven useful in topics like the nano-engineering of construction materials, correcting graphene planar defects, studying self-assembling bio-materials, and the densification, consolidation, and sintering of nanocrystalline materials.

## Keywords

Materials Science and Engineering, Nanotechnology, Molecular Dynamics

## 1. Introduction

Imagine witnessing the transformation of raw materials into molten metal in front of a roaring furnace. The intense heat, at immense temperatures, fuses the atoms, producing a substance with special applications and unique properties. This mesmerizing process has its roots in material science, which underscores the understanding of the intricate nature at the atomic level, which is also needed when developing new materials. The essence of such phenomena is not in our field of perception, as it takes us down to a level so trim that it's impossible to see. However, there has been a rise in computational methods that aid as a solution to this issue. One such way is called molecular dynamics.

Molecular dynamics (MD) is a simulation method used to explore the behavior of molecules and atoms. Molecular dynamics utilizes Newtonian, Lagrangian, or Hamiltonian mechanics to model specific behaviors and properties of atoms and particles. This simulation technique is an interdisciplinary technique

of research found across a wide range of scientific fields, used for studying, research, and innovation. MD also has applications in nanotechnology – you can also find heavy usage of materials science abstractions here. Nanotechnology is also a field by itself, but this paper will discuss the application of MD to nanotechnology, alongside the MD applications to materials science and engineering since there are plentiful intersections between them.

## 2. MD: Materials Science and Engineering

Materials Science and Engineering Materials science and engineering are fields that are important to certain industries. Materials science is a growing field that focuses on the research, design, and development of materials [1]. To make a device or structure, the erudition of its composition and the purpose of its behavior is crucial [2]. Materials scientists work with metals, polymers, ceramics, liquids, and composites. The studies of these materials find use in various other fields, such as biotechnology, nanotechnology, and electronics [3]. The research and development of making new materials is intricate for the learner who studies these fields. The main building blocks of materials are atoms of which the microscopic behavior leads to emergent macroscopic features [4]. The understanding of microscopic behavior is a necessity because it determines what happens in the macroscopic field of perception.

Molecular modeling, a way to model and describe molecules' generation, manipulation, and formation, quickly became a staple in these fields as new computational methods gained publicity. For example, simulations in material physics are a growing tool focused on studying lattice and defect dynamics [4]. Performing material simulations with MD is also a tool for innovation [4]. Technological innovation will lead to technological advancements, and MD is marketed as a tool for understanding, developing, and advancing these fields. MD simulations are effective computational experiments that characterize material properties and their responses [5].

### 2.1. Construction Materials Nano-Engineering

Molecular dynamics is utilized by nano-engineering, a discipline that falls under the branch of nanotechnology. Nano-engineering is a field that deals with nanomaterials, nanostructures, and nanoparticles. This branch falls under the broad study of nanotechnology and the umbrella of materials science and nano-engineering. Breakthroughs have occurred over the past decades concerning investigations of intricate phenomena of materials systems [5]. Previous studies have utilized computational methods, such as molecular dynamics to aid in the research and development of construction materials.

Construction materials are used to build essential civilian products, making it an important industry. The durability and mechanical behaviors of construction materials have become a growing concern as we depend on them in our daily lives [5]. The combination of computational methods of enhancement has luckily been proven effective. The perspective of the nano-scale with computational

methods like molecular dynamics is employed for the comprehension of the in-depth properties of these materials [5]. Molecular dynamics comes in and can then help correct any deformations with the help of molecular modeling and studying emergent properties, as material deformation always arises on the atomistic scale [5].

### 2.2. Semiconductor Research: Correcting Graphene Planar Defects

Molecular dynamics is used in the research and development of semiconductor materials. Semiconductor materials are a specialty within materials science and engineering. A semiconductor is a type of material used in the development of electronics because of its conduction properties. Defects in these materials have been an issue due to the necessity of their performance being optimal in electronics [6]. The performance of the semiconductors is dependent on their formation and defects will only hinder them.

Graphene is a material being considered on the rise when making semiconductors because of its electrical, optical, thermal, and mechanical properties [6]. Dealing with graphene, however, has also been a challenge due to grain boundary defects [6]. A grain boundary in materials science is a barrier between two "grains" or crystallites. Due to the scale of these planar defects, it is challenging to visualize experimentally under *in situ* graphene growth [6]. In situ growth, meaning growth in its original place. MD simulations successfully assisted with the research of grain boundary formations of graphene growth on copper by indicating that these boundaries are commonly found in 5 to 7-member carbon rings through molecular modeling [6]. In inclusion to that notion, molecular dynamics brought the scale to a visible playing field.

### 2.3. Biomaterials: Studying Self-Assembling Peptides

In materials science, biomaterials are materials solely for interacting with biological systems. Biomaterials are an essential part of biotechnology, where biotechnology is an integral part of nanotechnology. Biotechnology has been advancing due to the extensive research on the development of these materials within bioengineering with the application of materials science. Molecular dynamics plays a role in understanding and modeling interactions alongside the modeling of the actual materials and their properties. The study of self-assembling biomaterials uses molecular dynamics to model their interactions, structure, and assembly. An example of a self-assembling biomaterial is self-assembling peptides, which are also polymers. The self-assembly of peptides is the process by which the atomic and molecular constituents of the polymer aggregate into low-dimensional or 3-dimensional ordered materials [7].

An example of a molecular dynamics simulation method used in the study of self-assembling peptides is called Spontaneous All-Atom Molecular Dynamics, a simulation method that involves identifying atomic positions for a molecular

system that includes multiple components and where Newton's equation is solved at specified temperatures and pressures [7]. The All-Atom MD technique helps to describe the spontaneous evolution of molecular systems and the time-dependent behavior of biomolecules [7]. When it comes to insights, multiple can arise due to an in-depth analysis of experiments made following the molecular dynamics technique. For example, the mechanisms leading to the formation of nanostructures [7]. Essentially, the evolution of molecular and biomolecular systems and the morphological formation of certain nanostructures is time-dependent and involves knowledge of the current and the change of atomic positions. Using Spontaneous All-Atom MD helps to baseline the process of researching the formation and evolution of molecular systems with precision.

### 2.4. Nanomaterials and Nanoparticles: Copper Sintering

Nanomaterials are materials that are unique in terms of their uses and the scale that they are presented in. They are found on the nanoscale, a realm so small and difficult to work with. The usage of molecular dynamics techniques and simulations in this area can include the simulation of the processes of densification, sintering, and consolidation. These processes are unique in the way they are used and conducted with respect to the nanostructures studied. Taking a look at the sintering of nanoparticles is an excellent choice for the analysis of the usage of molecular dynamics.

A study done using molecular dynamics explored the effects of pressure-assisted sintering on the kinetic thermal and mechanical behaviors of the copper nanoparticles used. LAMMPS was used to perform all of the simulations [8]. LAMMPS stands for Large Scale Atomic/Molecular Massively Parallel Simulator. It is mainly focused on material modeling. As a result of the study, they collected information related to the effects of different pressures and temperatures when it comes to pressure-assisted sintering. According to the study, they analyzed the plotted displacement vectors of which the simulated sintering occurred under 100 and 300 MPa [8]. Through the resulting data analysis that resulted from the simulation processes, they concluded that through the increase of external pressures, the plastic flow is more intensive between the specific copper nanoparticles while also affecting the defects generation during sintering [8]. Higher pressure leads to higher coalescence [8]. Coalescence is the merging of elements to form a larger mass, which has a direct relationship to pressure, meaning that the higher the pressure, the higher the ability to coalesce between the materials. It is also important to take into account the idea that the generation of defects is also in a direct relationship with increased pressure. Important details like these can be further analyzed theoretically with the use of molecular dynamics.

The atomic trajectories were also analyzed in accordance with the effect of temperatures on the system. The trajectories of the atoms that were simulated under 300 K and 500 K were plotted [8]. The temperatures of systems that were

simulated were assisted with both pressure and without pressure. Details and relationships were recorded that analyzed any similarities or differences. The initial information from the study collected stated that the atomic migration for both of the different temperatures was relatively the same when done at 300 K and 500 K and that atoms were able to migrate around pressure defects at each of the temperatures [8]. While the atomic migration was seemingly the same, a further depth analysis was conducted that showed the true effect of temperature when the simulation time was adjusted. At 500 ps, the differences in the performances of the temperatures in relation to atomic migration were recorded [8]. A thorough analysis of this segment of the experiment can be linked with the effectiveness of molecular dynamics.

The study assessed and others like it are able to reveal the contribution of molecular dynamics methods. The investigation of the previously mentioned study not only shows a profound analysis and understanding of pressure-assisted densification but also underscores the usage of molecular dynamics in this area of study. The simulation technique of molecular dynamics is a very powerful tool for studying the nanoscale and the analysis of certain processes like the sintering of copper nanostructures. The importance of experimentation can take the usefulness of molecular dynamics as a stepping stone to achieve even more development in this branch.

## 3. Conclusion

The merging of computer science and other fields has given birth to remarkable tools of research and innovation. Molecular dynamics simulations have been employed in various fields and have primarily been proven useful in materials science and engineering and nanotechnology. Unique progress has been made in places where it may have not been possible without this simulation method. There has been progress witnessed with the enhancement of research using the molecular dynamics technique in certain areas that tend to intersect with the applications of materials science, like nanotechnology and nano-engineering, biotechnology and bioengineering, and electronics. Biotechnology itself is also an integral part of nanotechnology.

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## Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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