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Article

Molecular dynamics simulation of the solidification process of magnesium alloy medical materials

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Abstract: The process of solidification, which includes the creation of ice, a liquid can become a solid by freezing solder in electrical circuits or casting metal in industrial settings. Magnesium alloys have developed as promising tools for biomedical applications due to their desirable properties such as low density, high strength, and excellent biocompatibility. These alloys are increasingly used in various applications and devices, where their performance is heavily influenced by their microstructure characteristics. The objective of the research is to establish a molecular dynamics simulation of the magnesium alloy medicinal material solidification process. Magnesium alloys widely recognized for their biocompatibility and biodegradability are increasingly used in medical implants. In this study, MD simulations are applied to represent the atomic interactions and microstructural development during the solidification process. During the solidification phase, the simulation advances, tracking the emergence and expansion of solid nuclei while varying cooling rates to investigate their effects on the dynamics of solidification. This research parameter, such as temperature variations, cooling rates, and phase transformations, is analyzed to reveal the nucleation and growth of solid phases. Two appropriate force fields that are used to explain the possible energy interactions between atoms are the modified embedded atom method (MEAM) and the embedded atom method (EAM). The findings shed light on the kinetics of crystallization and the impact of alloy composition on solidification behavior. This study provides useful suggestions for improving the performance and dependability of magnesium alloys in biomedical equipment.

Keywords: molecular dynamics; solidification process; magnesium alloy; medical implant

1. Introduction

The unique combination of mechanical properties of magnesium alloys makes them very popular in the fields of medical technology, biocompatibility, and biodegradability [1]. Due to its lightweight, magnesium is the most preferred structural metal for tasks where reducing the weight of medical equipment is crucial. It also has a high strength-to-weight ratio [2]. Also, magnesium alloy is quite biocompatible since magnesium is present in the human body at a reasonable concentration and is involved in several biochemical cycles [3]. Eventually, such magnesium-based implants could be absorbed by the body in the situation, hence not requiring a secondary operation to extract the device, which has contributed to its popularity in providing temporary implants like stents, orthopedic devices, and vascular pasture [4]. **Figure 1** shows the magnesium alloy in medical materials.

Figure 1. Magnesium alloy in medical instruments.

Solidification plays a critical role in the manufacturing of magnesium alloy biomaterials since it governs the greatest mechanical characteristics and microorganisms of the substance [5]. While solidifying, the growth of grains, dendrites, and other microstructural features thereby affects the strength, ductility, and wear of the alloy [6]. Therefore, increasing the qualities of magnesium alloys for medicinal purposes requires an understanding of the atomic-level solidification process [7]. It is especially true because the cooling rates and processing conditions are different for magnesium alloys and these directly affect the microstructure, resulting in the performance differences [8].

At the atomic level, MD has risen as a powerful instrument for examining metals and alloy solidifying processes. Through the simulation of interactions between individual atoms, MD simulations can yield detailed information about nucleation and growth of crystalline structures during solidification [9]. MD simulations might provide a more profound understanding of atomic-scale interactions that alter microstructural features, leading to changes in the automated and corrosion properties of magnesium alloys [10]. Therefore, such knowledge would help develop novel magnesium alloys suitable for medical applications with improved performance.The objective of the research is to establish a molecular dynamics simulation of the magnesium alloy medicinal material solidification process.

The structure of this work is as follows: Related work is presented in Part 2. Part 3 describes the simulation setup. The results and discussions are presented in Part 4 and the study is concluded in Part 5.

2. Related work

Employing a molecular dynamics technique, Kundu examined how thermal process parameters affected the alloying of $Al-10Mg$ systems [11]. For the purpose of melting, combining, and cooling Al and Mg nanoparticles, five heating rates were to be taken into consideration. The investigation discovered that heating rates had a major impact on the melting temperature of component NPs. The findings

revealed a small impact on mechanical properties but a strong correlation between temperature rise and convergence kinetics.

In Al-Mg-based alloys, MgO particles might serve as possible nucleation sites during the solidification process. Fang examined the effect of MgO materials on atomic arrangement in fluid Al within the liquid Al/solid MgO connections to operate employing an AIMD method [12]. The results indicated that at thermal equilibrium, the O-terminated MgO surface developed an Al-terminating layer with vacant positions leading to essential toughness. In liquidAl, both Mg-terminating and $MgO-0.01$ substrates remain stable.

Utilizing nonequilibrium molecular dynamics simulations, Jiang examined the effects of vacancies on spallation and dynamic response in single-crystal Mg [13]. The findings indicated that spall damage was greatly impacted by situation deficiencies, while the effects on compression-induced plasticity in the [0001] direction were minimal. In the [10–10] direction, they lessened spall damage and offered nucleation sites for compression-induced plasticity. The investigation also looked at the way excellent and defective magnesium vary in spall strength at various shock velocities.

Amorphous alloys with distinct mechanical properties and structures made bulk metallic glasses. Barik investigated the glass-forming ability and structural evolution of $Zr50Ag50$ alloy during solidification using MD simulations with MEAM parameters [14]. Methods such as coordination number transportation, Voronoi tessellation analysis, and radial distribution functions were applied. Good glass-forming ability was indicated by the lower glass transition temperature. The formation of the majority of metallic glass in the alloy was confirmed by the larger population of icosahedral structures revealed by the Voronoi tessellation assessment.

The primary goal of an economical way to fix broken components and get them back to working order was through additive manufacturing. Chen examined the mechanical characteristics and microstructures of polycrystalline Ti that had undergone post-polishing and PBF repair due to surface damage [15]. The findings demonstrated that, in comparison to grain interiors, GBs in Ti were more vulnerable to temperature elevation damage. Due to an increased capacity for carrying dislocations, 96.8% of the yield capacity of perfecting specimens was recovered from damaged samples by applying PBF repair and post-polishing therapy. Because of more arranging problems and twins, the flow stress was higher than in perfect samples.

Pesode focused on materials, microscopic structure, mechanical properties, biocompatibility, decomposition, and antibacterial qualities while examining various AM techniques for producing medical devices from magnesium-based alloys [16]. Although selective laser melting offered more functionality than selective laser sintering because of the deep penetration of magnesium, PBF was found to be an effective method. The design, features, and applications of bioimplants were highlighted in the article along with the difficulties and issues related to AM techniques.

Die-casting products were one of the many applications for magnesium alloys, an environmentally friendly engineering material. However, Li produced a large

amount of waste, which contaminated secondary resources and the environment [17]. A low-pressure distillation-directed evaporation study found that under some conditions, the level of purity may exceed 99.98% and the magnesium volatilizing produced could reach 93.76%. The research stipulated a conceptual and operational basis for the low-pressure distillation technique for recuperating waste magnesium alloy.

A novel alloy design strategy was presented in Gao to speed up the search in highly dimensional framework space for hypoeutectic $Al-Si-Mg-Sc$ circulation alloys [18]. High-throughput solidification simulations using CALPHAD were used to determine the quantitative relationship between microstructure, process, and composition. Using the participatory learning technique, it was possible to determine the connection between the microstructure and mechanical characteristics of $Al-Si-Mg-Sc$ hypoeutectic circulating alloys. Extending the strategy to filter the optimal $Si, Mg, and\ Sc$ contents over the high-dimensional hypoeutectic $Al-xSi-yMg-zSc$ structure environment was effective.

HEAs were renowned for their mechanical qualities and appealing microstructures. Nguyen used MD simulation and ML to study the process of deformation of $AlCoCrCuFeNi$ HEAs under various circumstances, such as temperature, velocity of strain, and particle proportions [19]. The MD simulations illustrate that shear groups follow the uniaxial tensile axis, with strain and temperatures being the highest bases of initial strain. The disconnection development mechanism indicated that dislocations nucleated around the grain's boundary under increased strain. The findings were validated by the ML prediction results, which closed the gaps between MD and ML and reduced the time, labour costs, and time required for HEA deformation testing in the real-world setting.

3. Simulation setup

Figure 2 shows the overall flow for solidification process. The framework will be based on a magnesium alloy, $Mg-Ca$ or $Mg-Zn$ for instance, containing between 100,000 and 1,000,000 atoms, depending on the required precision and the available computational resources. **Figure 3** then instructs the replacement of the corresponding magnesium atoms.

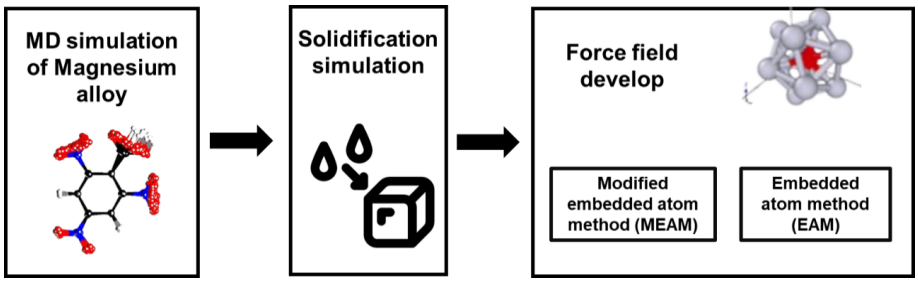

Figure 2. Overall flow.

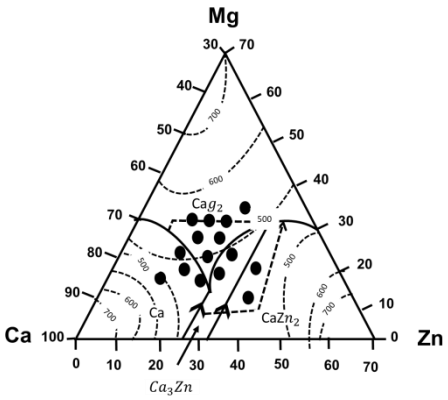

Figure 3. Magnesium atoms.

At first, the atoms will be placed in random order to resemble a high-temperature liquid, beginning from approximately $1200\,K$ that is higher than magnesium alloys' melting temperature. A cubic or rectangular simulation box will be used, but PBC will be applied in all three directions to create the illusion of an infinite system, thus preventing any edge effect and allowing for sufficient thermal expansion and contraction during the cooling process. **Table 1** shows the simulation setup.

Table 1. Simulation setup.

Parameter	Values/Settings
Material	Magnesium alloy (e.g., $Mg-Ca$, $Mg-Zn$)
Number of atoms	100,000–1,000,000
Simulation box	Cubic/Rectangular, Periodic Boundary
Force fields	MEAM, EAM
Initial temperature	1200 K
Cooling rates	1 K/ps (slow), 10 K/ps (fast)
Final temperature	300 K (or lower)
Ensemble	NPT (Nosé-Hoover or Langevin thermostat)
Time step	1– 2 fs
Total simulation time	1– 10 ns
Equilibration time	100– 200 ps

In this study, both the MEAM and the EAMare employed to capture the essence of metallic bonding and effects of alloying within parameters that are valid for the range of temperatures of interest.

1) The EAM potential is particularly useful for simulating the pairwise interactions of atoms in metallic systems. It takes into consideration the energy generated by surrounding atoms, which is essential to effectively modelling the bonds in metals and alloys. This potential is especially useful for systems where the electrical structure plays an important role in bonding, such as magnesium alloys.
2) The MEAM improves on the EAM technique by introducing angular dependency into atomic interactions. This enables a more detailed description

of the atomic environment, which is critical for understanding the impact of alloying elements on mechanical characteristics and phase transitions in magnesium alloys. The capacity to simulate angular interactions is essential in comprehending the complicated dynamics of solidifying phenomena.

To determine the pairwise interaction between a metal and its alloy, one commonly uses the EAM potential. The potential of the MEAM can be appropriate for modeling metals and alloys in addition to computing the pairwise interactions of different materials.

The cooling process will involve two different rates: slow cooling rate with a value of $1\ \mathrm{K/ps}$ for a near equilibrium solidification and fast cooling rate with a value of $15\ \mathrm{K/ps}$ for rapid solidification, all aiming at achieving a final temperature of about $300\ \mathrm{K}$ or below. The temperature will be kept constant using a Nosé-Hoover or Langevin thermostat in an NPT ensemble that also keeps number of particles as well as pressure and temperature constant. The complete simulation time will not be less than 1 nanoseconds and more than 10 nanoseconds with intervals of 1 to 2 femtoseconds to take account of the transistor atoms even in motion. Before actually cooling the system down, an initial equilibration stage of 100 to 200 picoseconds will be offered at deliberately higher temperature to settle the system.

Throughout the entire simulation, the formation of solid nuclei will be assessed through a measurement of the cluster populations, while the examinations of microstructure, particularly for crystalline structures and imperfections, will be focused on CNA and RDF. In order to separate solid and liquid phases, the potential energy per atom or local order parameters will be used. In addition to that, the data collection will involve recording total, potential and kinetic energy, performing structural analysis of the atomic arrangement and grain boundary using Voronoi tessellation and bond-angle analysis techniques among others.

To ensure effective implementation, the molecular dynamics simulations will be performed with the aid of LAMMPS or GROMACS software on HPC clusters to allow for large system sizes and long simulation durations. OVITO and other tools of a similar kind will be used to generate the atomic arrangements and monitor the solidification process. This entire configuration is intended to extend the understanding of phase transformation and microstructure evolution of magnesium alloy based biodegradable implants at variable cooling rates.

4. Results and discussion

The simulation of a magnesium alloy (for example, $Mg - Ca$ or $Mg - Zn$) was used, it is important to discuss temperature variations as they help in the solid transitions of the liquid material ($1200\ \mathrm{K}$ in this case) as the figureheads cooling. The cooling rates ($1\ \mathrm{K/ps}$ for slow cooling and $15\ \mathrm{K/ps}$ for fast cooling) play a major role in the generation of structures during and after solidification. For this purpose, phase transformations are registered that help to trace a liquefied material turning into a solid one using potential energy and local order parameters of phases, aiding in understanding the inner structure development of bioresorbable implants that are phase Mg wrought alloys.

4.1. Temperature variations

Temperature variations are the changes in temperature concerning the time elapsed during the cooling and solidification cycle, thus affecting the thermal energy available for the motion and interaction of atoms. In this case, temperature variations are controlled to study how they affect the nucleation and solidification of magnesium alloys. It is anticipated that lower temperatures will increase the rate at which nucleation occurs and affect the structure of the solidified component. **Figure 4** and **Table 2** show the nucleation behavior at different temperatures.

Table 2. Effect of temperature variations on nucleation and growth.

Temperature (K)	Number of Nuclei	Average Nucleus Size (nm)	Crystallization Time (ns)
1200	150	5.0	5.0
1100	300	10.2	4.0
1000	450	15.8	3.0
900	600	20.0	2.0
800	800	25.3	1.5

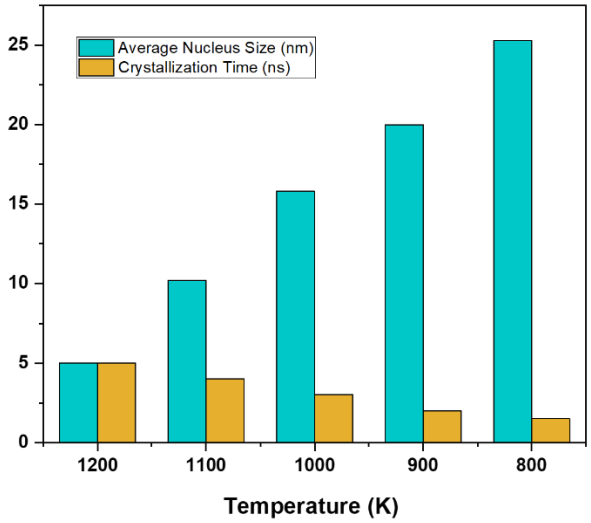

Figure 4. Average nucleus size, crystallization time at temperature variations.

Temperature variations affect nucleation and growth by influencing atomic mobility and energy distribution. At higher temperatures, atoms have more thermal energy, leading to slower nucleation but larger crystal structures due to extended atomic diffusion. As temperatures decrease, reduced atomic movement accelerates nucleation, resulting in faster solidification and smaller, more numerous nuclei, similar to how water freezes faster at colder temperatures, forming smaller ice crystals.

4.2. Cooling rates

The term cooling rates denotes the rate of heat loss of a substance; however, this is often simplified in praise of the degrees lost per second (K/s *or* K/ps). The different cooling rates are experimented on in the current research to analyze how

they influence the solidification processes of magnesium alloys. In turn, lower cooling rates give an extended period for nucleation and growth without any disturbances, whereas higher rates can produce finer microstructures leading to different mechanical properties. **Figure 5** and **Table 3** show the cooling rates.

Table 3. Impact of cooling rates on solidification dynamics.

Cooling Rate (K/ps)	Average Nucleus Size (nm)	Number of Nuclei	Crystallization Time (ns)
1	25.3	900	5.0
5	18.6	750	3.0
10	12.0	600	2.0
12	10.5	550	1.8
15	8.5	500	1.5

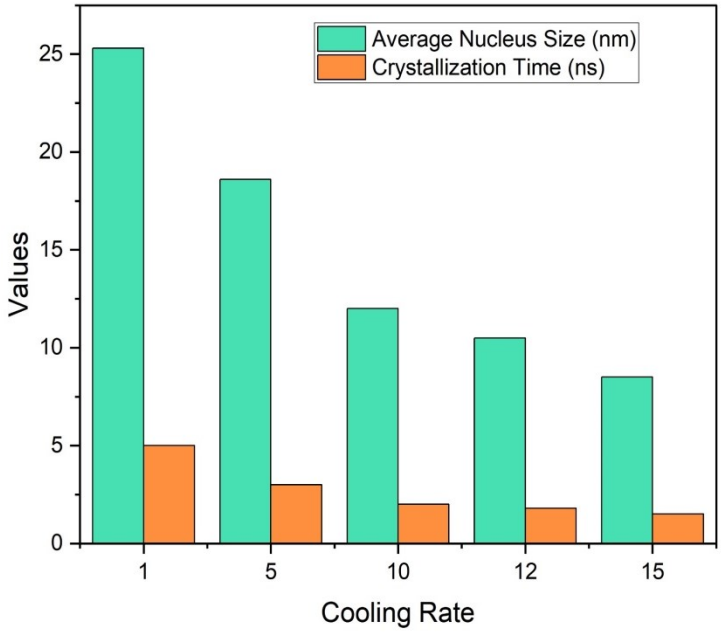

Figure 5. Average nucleus size, crystallization time at cooling rate influence.

4.3. Phase transformations

Phase transformations are changes in the state of matter during the process of heating or cooling and solidifying, for example, from liquid to solid. It focuses on such phase transformations when cooling to analyze the solidification mechanism of magnesium alloys. It also aims to follow the liquid-to-solid phase transition to devise the best conditions under which materials with suitable mechanical characteristics can be synthesized. **Table 4** shows the phase transformations.

Table 4. Phase transformation data during cooling.

Cooling Rate (K/ps)	Initial Phase	Final Phase	Transformation Time (ns)
1	Liquid	Solid	5.0
5	Liquid	Solid	3.0
10	Liquid	Solid	2.0

4.4. Discussion

The solidification process of magnesium alloys is simulated using molecular dynamics in this study, with special focus to the microstructural characteristics used in the biomedical industry. Simulation of magnesium alloys such as Mg-Ca and Mg-Zn shows that the temperature variations and cooling rates have a significant impact on solidification processes, decreasing the temperature from 1200 K to 800 K increases the number of nuclei from 150 to 800 and reduces the average nucleus size from 5.0 nm to 25.3 nm which suggests that faster nucleation occurs at lower temperature. This is shown in cooling rates to give an average nucleus size of 25.3 nm and crystallization time of 5.0 ns at 1 K/ps, 12.0 nm and 2.0 ns at 10 K /ps indicating finer microstructures sampled with rapid cooling. Additionally, the transformation time for the liquid-to-solid phase transition decreases from 5.0 ns at 1 K/ps to 2.0 ns at 10 K/ps, highlighting the acceleration of solidification with increased cooling rates. These findings emphasize the importance of controlling temperature and cooling rates to optimize the microstructural characteristics of magnesium alloys for biomedical applications.

The results were supplemented by the utilization of force fields such as the MEAM and EAM, where the atomic interactions were well modeled for accurate simulation results. The process of solidification affected the mechanical properties of magnesium alloys because slower cooling increased both ductility and yield strength owing to large, well-defined microstructures whereas faster cooling led to smaller grains that have increased strength at expense of potential loss in ductility. In other words, the attributes should be balanced to increase the performance of magnesium alloys in vivo in biomedical applications where magnesium alloys should stabilize under physiological stresses yet still flexible enough to accommodate deformation. These magnesium alloys do present some unique challenges in biomedical applications; this is because of their susceptibility especially towards corrosion in vivo and to rapid degradation in physiological environments, which may create a premature loss of mechanical integrity and thus potential complications of the performance of the implants. Although their potential for biodegradability and biocompatibility has made them interesting for applications in transients, implants, controlled degradation rates may facilitate tissue healing. Notably, the avoidance of secondary surgery turns them into excellent candidates for bone fixation devices and scaffolds in regenerative medicine applications. The findings of this research help to emphasize the need for magnesium alloy optimization in biomedical practices while acknowledging the limitations of the current mechanical understanding and exploration of complex alloy systems that will improve the solidification and performance of materials in biomedical applications.

5. Conclusion

Study successfully developed a molecular dynamics computational approach to understanding the solidification of magnesium alloys. Application in biomedical areas is on the rise because of its low density and high strength coupled with good compatibility with the human body. This research, in particular, uses MD simulations to model the atomic events at high temperatures and how the system

develops microstructure during solidification, specifically the formation and growth of solid nuclei at different cooling rates. Temperature, cooling rates, and phase change, among others, were found to be significant in explaining nucleation and growth processes and growth. The use of MEAM and EAM force fields enabled a better understanding of an interaction energy between atoms. Such results elucidate the crystallization kinetics and how such kinetics are influenced by alloy composition in solidification, which can be used to develop the performance and reliability of magnesium alloy for medical implants and devices.

Author contributions: Conceptualization, YY and YF; methodology, SY and CQ; software, JL and CQ; validation SY and JL; writing—original draft preparation, YY; writing—review and editing, YF. All authors have read and agreed to the published version of the manuscript.

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Conflict of interest: The authors declare no conflict of interest.

Abbreviations

molecular dynamics = MD

modified embedded atom method = MEAM

embedded atom method = EAM

Magnesium = Mg

titanium = Ti

powder bed fusion = PBF

grain boundaries = GBs

Additive manufacturing = AM

Calculation of PHAse Diagrams = CALPHAD

High-entropy alloys = HEAs

periodic boundary conditions = PBC

large-scale atomic/molecular massively parallel simulator = LAMMPS

high-performance computing = HPC

radial distribution functions = RDF

common neighbor analysis = CNA

nanoparticles = NPs

Ab initio molecular dynamics = AIMD

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