Analysis of Nucleation Characteristics and Grain Growth Dynamics in Aluminum and Its Titanium Alloys: A Molecular Dynamics Simulation Study on Critical Nucleus Size, Nucleation Rate, and the Effects of Growth Restriction Factors Based on the MFPT Method

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ABSTRACT: This study utilized LAMMPS molecular dynamics simulation software and the Mean First-Passage Time (MFPT) method to systematically analyze the dynamic behavior of nucleation and grain growth in aluminum (Al) and its titanium (AlTi) alloys. Initially, the research calculated the critical nucleus size, nucleation rate, and grain growth rate for Al. Subsequently, the impact of Ti addition on these parameters was investigated, particularly under various growth restriction factor conditions. The results indicated that the addition of Ti significantly reduced the nucleation rate, critical nucleus size, and grain growth rate of the aluminum alloy. Furthermore, an increase in the growth restriction factors further decreased the nucleation rate, critical nucleus size, and grain growth rate.

Keywords: Growth restriction factors ; Molecular dynamics simulation ; Critical nucleus size ; Nucleation rate

1 Introduction

The properties of metal alloys, such as aluminum and its composites, are largely determined by their nucleation and subsequent grain growth during solidification. These properties in turn critically influence the mechanical behavior and durability of the resulting materials.

Molecular dynamics (MD) simulations have emerged as a powerful tool for exploring these phenomena on an atomic scale, providing detailed insights that are often inaccessible through conventional experimental approaches. This study employs the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), a sophisticated MD simulation software, to investigate the dynamics of nucleation and grain growth within pure aluminum and its titanium alloys (AlTi).

The inclusion of titanium in aluminum alloys is widely recognized for its potential to enhance material properties through microstructural refinement. However, the mechanisms by which Ti influences nucleation and grain growth in aluminum alloys are not fully understood and require detailed investigation. To this end, our research utilized the Mean First-Passage Time (MFPT) method to systematically quantify the critical nucleus size, nucleation rate, and grain growth rate in these alloys.

Initial simulations focused on pure aluminum to establish baseline measurements of nucleation and grain growth dynamics. Subsequent simulations introduced titanium into the aluminum matrix, and the effects of Ti on these parameters were thoroughly analyzed. The study specifically examined the role of growth restriction factors, which are crucial in controlling the microstructural evolution during solidification.

Our findings revealed that the addition of titanium significantly reduces the nucleation rate, critical nucleus size, and grain growth rate in aluminum alloys. Moreover, increasing the growth restriction factors further diminished these parameters, suggesting that Ti addition and the manipulation of growth restriction conditions could be strategically used to enhance the performance of aluminum alloys. This study not only contributes to a deeper understanding of the solidification processes in Al-Ti alloys but also offers practical insights for the development of advanced materials with improved mechanical properties.

2 Experimental procedure

The MD simulations were conducted using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software (Sandia National Laboratories, Livermore, California, USA). In this work, the pure aluminum simulations were performed using a box containing 171,500 FCC lattice atoms in a 141.75 Å×141.75 Å×141.75 Å box; the aluminum-titanium alloys were also simulated using a box with 171,500 FCC lattice atoms of the same dimensions. The models were divided into two groups with different growth restriction factors, containing 48,123 and 39,565 titanium atoms, respectively. The study used the EAM potential. Periodic boundary conditions were applied in all three dimensions, with an integration timestep of 5 fs. The simulations applied an isothermal-isobaric ensemble (NPT), with temperature controlled via a Nosé-Hoover thermostat and pressure controlled by volume scaling. Due to the limited spatial and temporal scales of MD simulations, and because nucleation in metal melts is a random event, independent runs are

necessary to obtain statistically meaningful results. In this study, each simulation was repeated five times.

Initially, the perfect single crystal of aluminum was heated from the solid state at 300 K to the liquid state at 2000 K. The liquid was then cooled to 300 K at a rate of 2.0×10^{11} K/s, and nucleation was observed during the cooling process.

For the aluminum-titanium model, the system was heated from 300 K in the solid state to 2000 K in the liquid state, and then relaxed at 2000 K for a period. The relaxed liquid alloy served as the initial state of the model and was cooled from 2000 K to 300 K at a rate of 2.0×10^{11} K/s. All simulations were conducted at 0 MPa pressure.

The microstructural evolution during solidification was observed using the visualization software OVITO. The local environment of atoms was determined using the Adaptive Common Neighbor Analysis (CNA) method. CNA determines the atomic structure by calculating the topology of each atom's nearest neighbors. By comparing the computed values to known characteristics of standard crystals, the local atomic crystal structure can be distinguished. In OVITO, atoms not identified as FCC, HCP, BCC, or any other crystalline type are classified as ICO liquid or ICO solid atoms.

Cluster analysis in OVITO was used to export plots showing the change in the internal atomic count of clusters over time, and the MFPT method was employed to calculate the critical nucleus size and nucleation rate for aluminum and aluminum-titanium.

The growth restriction factor was calculated with reference to the article "Growth Restriction Factor in Al-Si-Mg-Cu Alloys" by Robert-Koch-Str.

3 Result and discussion

The molecular dynamics simulations provided comprehensive insights into the effects of titanium addition and growth restriction factors on the nucleation and grain growth dynamics in aluminum and its titanium alloys.

(1) Nucleation Rate and Critical Nucleus Size: Initial results indicated that titanium addition significantly reduces the nucleation rate and the critical nucleus size in aluminum alloys compared to pure aluminum. The titanium addition enhanced the growth restriction factor, thereby creating a solute-rich environment that hinders nucleation. The Mean First-Passage Time (MFPT) method was used to quantify the nucleation rates and critical nucleus sizes, confirming that as titanium content increases, the nucleation rate decreases due to higher solute concentrations impeding nucleation. The critical nucleus size also reduced, implying that smaller nuclei become stable with titanium addition.

(2) Grain Growth Rate: Titanium's presence in the aluminum matrix also had a marked effect on the grain growth rate. With the increased concentration of titanium, the grain growth rate decreased. This is attributed to the growth restriction factors created by titanium, which inhibited the growth of existing grains. The results demonstrated that higher concentrations of titanium significantly slow the grain growth rate.

(3) Growth Restriction Factors: By analyzing models with varying growth restriction factors, the results showed a clear correlation between an increase in growth restriction factors and a further reduction in nucleation rates, critical nucleus sizes, and grain growth rates. This reinforces the concept that manipulating growth restriction factors via alloying elements like titanium provides a strategic approach to refine microstructure and improve the properties of aluminum alloys.

(4) Implications: These findings underscore the importance of growth restriction factors in the solidification behavior of aluminum-titanium alloys. The strategic addition of titanium, along with optimized growth restriction factors, offers a pathway to designing advanced aluminum alloys with refined microstructures and superior mechanical properties. Further studies should focus on validating these findings through experimental work and exploring the applicability of different alloying elements in other metal matrices.

4 Conclusion

The addition of Ti significantly reduced the nucleation rate, critical nucleus size, and grain growth rate of the aluminum alloy. An increase in the growth restriction factors further decreased the nucleation rate, critical nucleus size, and grain growth rate.