Proceedings of CONF-MPCS 2025 Symposium: Leveraging EVs and Machine Learning for Sustainable Energy Demand Management
DOI: 10.54254/2753-8818/2025.GL24106

Research Progress on the Integration of Molecular Dynamics and Machine Learning in 3xxx Series Aluminum Alloys

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Abstract: With the increasing demand for high-performance materials in transportation, construction, and electronics industries, the need for efficient and precise alloy design has become more critical. This study focuses on the integration of molecular dynamics (MD) simulations and machine learning (ML) techniques in the research and optimization of 3xxx series aluminum alloys. The primary objective is to explore how the combination of these two methods can enhance the understanding of micro-mechanisms and accelerate alloy design processes. The research adopts a comprehensive literature review approach, analyzing existing experimental studies, simulation results, and machine learning applications related to 3xxx series alloys. Key tools include molecular dynamics simulation for atomic-scale behavior analysis and machine learning models for property prediction and optimization. The study finds that integrating MD and ML significantly improves the efficiency of data analysis, performance prediction, and microstructure control in 3xxx series alloys. It concludes that the MD-ML hybrid approach offers a promising path to address traditional limitations in alloy research and paves the way for the intelligent design of advanced aluminum materials.

Keywords: 3xxx series aluminum alloys, molecular dynamics, machine learning, alloy design

1. Introduction

Due to their excellent specific strength, corrosion resistance, and workability, aluminum alloys are widely used in transportation, construction, and electronics industries. Among them, 3xxx series aluminum alloys (primarily Al-Mn-based alloys) are notable for their outstanding corrosion resistance and weldability, making them ideal for applications such as beverage cans, automotive body panels, and architectural decorations [1]. However, as industrial demands for material performance continue to rise, traditional alloy design and optimization methods are increasingly exposing limitations such as low efficiency and lengthy development cycles.

In recent years, molecular dynamics (MD) simulations have become an important tool for understanding the microscopic mechanisms of materials and revealing atomic-scale behaviors [2]. Meanwhile, machine learning (ML), as an effective approach for handling complex and high-dimensional data, has shown great potential in materials science, particularly in material design, performance prediction, and data mining [3]. The combination of MD simulations and ML methods is expected to break the limitations of traditional techniques and open up new pathways for studying 3xxx series aluminum alloys.

This paper reviews the progress in the integration of molecular dynamics and machine learning in 3xxx series aluminum alloys, covering aspects such as micro-mechanical behavior simulation, alloy

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design optimization, and corrosion mechanism exploration, and analyzes the current challenges and future development prospects. This study not only provides new insights into improving the performance and extending the service life of traditional 3xxx series aluminum alloys but also lays a foundation for promoting the application of lightweight materials in industries such as transportation and construction. Additionally, the methodologies summarized in this paper offer important references for researchers engaged in intelligent design and performance prediction of aluminum alloys and other metallic materials, providing theoretical support and technical guidance for the development of next-generation high-performance alloys.

2. Experimental research on 3xxx series aluminum alloys

3xxx series aluminum alloys, with manganese (Mn) as the primary alloying element, exhibit good corrosion resistance and formability. Common grades include 3003, 3004, and 3105. Their strength is mainly achieved through solid solution strengthening and work hardening, without the possibility of heat treatment strengthening (unlike 2xxx or 7xxx series) [1]. Therefore, the potential for mechanical property enhancement in 3xxx series alloys is limited, requiring optimization through composition adjustment and microstructure control.

In previous studies, researchers have explored the mechanical properties, corrosion behavior, and microstructural evolution of 3xxx series aluminum alloys through traditional experimental methods.

First, regarding mechanical properties, Zhang et al. processed 3003 aluminum alloys using cryogenic rolling (CR) and room temperature rolling (RTR) techniques to investigate the relationship between microstructure, texture evolution, and strengthening mechanisms. The results showed that cryogenic rolling significantly refined subgrains and second-phase particles, increased dislocation density, and improved yield strength, tensile strength, and elongation. The primary strengthening mechanisms were dislocation strengthening and grain refinement [4].

Second, in terms of corrosion resistance, Zamin conducted systematic studies on the effect of Mn content on the corrosion behavior of Al-Mn alloys through corrosion tests and metallographic analysis. It was found that increasing the Mn/Fe ratio reduced the potential difference between the aluminum matrix and intermetallic compounds, significantly improving corrosion resistance. Furthermore, the addition of magnesium (Mg) had little impact on corrosion behavior. This study explained the beneficial role of Mn from the perspective of micro-electrochemical mechanisms [5].

Third, concerning microstructure and texture evolution, Kao investigated the effects of cold rolling and annealing on the texture evolution and "earing behavior" of 3004 aluminum alloys. X-ray diffraction analysis revealed that cold rolling and subsequent annealing significantly altered the crystallographic orientation distribution. Specifically, the difference in X-ray intensity between the (422) and (200) planes was highly correlated with the formation of 45° ears, and variations in the intensity of (111) planes influenced the evolution of earing angles. This study provided experimental insights into the relationship between texture evolution and formability in 3xxx series alloys [6].

3. Typical applications of molecular dynamics in 3xxx series aluminum alloys

Although experimental research has uncovered many performance characteristics of 3xxx series aluminum alloys, understanding the physical mechanisms at the atomic scale remains challenging due to experimental limitations. Molecular dynamics simulations provide an effective means to explore material behavior and structural evolution from a microscopic perspective. This section introduces several typical application areas of MD simulations in 3xxx series alloys.

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3.1. Mechanical properties

During the processing of aluminum alloys, such as cold rolling or tensile deformation, a large number of dislocations are generated and move. MD simulations can accurately depict the structural evolution of dislocation cores, slip mechanisms, and interactions with other defects. For example, Kuksin et al. investigated the dynamic behavior of edge dislocations in pure aluminum through MD simulations, revealing the migration speed, expansion mechanisms, and slip plane transitions under different stress loading conditions [7].

3.2. Corrosion behavior

Grain boundaries are the main vulnerable regions for corrosion in aluminum alloys, particularly in chloride environments where localized corrosion is prone to occur. Ab initio molecular dynamics (AIMD) and density functional theory (DFT) simulations have been employed to study the initial stages of chloride adsorption and corrosion at alumina grain boundaries. Sundar et al. constructed hydroxylated α-Al_2O_3 single-crystal and bicrystal models and studied substitution reactions between Cl^- ions and surface hydroxyl groups in aqueous environments. The results indicated that Cl^- ions could form stable adsorption only near grain boundaries, initiating localized corrosion by promoting the dissolution of Al^{3+} into the electrolyte [8].

3.3. Phase formation and evolution

The Al_6Mn second phase, commonly observed in 3xxx series aluminum alloys, significantly influences mechanical properties and corrosion behavior. Although experimental observations have suggested its importance, its three-dimensional morphology and growth mechanisms remain unclear. Wang et al. established a phase-field model based on crystallographic orientation relationships, lattice matching, and transformation strain to simulate the nucleation, growth, and morphological evolution of Al_6Mn precipitates. Their results revealed that the morphology of Al_6Mn precipitates is size-dependent, evolving from equiaxed to prismatic or plate-like shapes as the size increases [9].

4. Current applications and prospects of machine learning in aluminum alloys

However, relying solely on MD simulations faces challenges such as high computational costs and limited parameter spaces. Therefore, machine learning (ML) methods have recently gained widespread attention in the field of aluminum alloys as efficient tools for processing complex data and enabling data-driven prediction and optimization.

Although ML applications in materials science are relatively new, their use in aluminum alloy research has expanded rapidly, encompassing mechanical property prediction, image recognition, corrosion modeling, and process optimization. Major application areas include:

a. Performance Prediction: Using existing experimental or simulation data to train models that predict mechanical properties such as yield strength, elongation, and hardness. Ensemble models like Random Forest and XGBoost have been effective in handling nonlinear composition-property relationships [10].

b. Corrosion Behavior Modeling: Establishing prediction or classification models based on composition and electrochemical environments (e.g., pH, Cl^- concentration) to evaluate corrosion risks under specific service conditions [11].

c. Image Recognition and Microstructure Analysis: Using convolutional neural networks (CNNs) to automatically identify microstructures, grain sizes, or precipitate distributions from SEM and EBSD images, enabling efficient and objective microstructural analysis.

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d. Thermal Processing Optimization: Predicting final microstructure and properties based on parameters such as annealing temperature, time, and deformation degree, thereby recommending optimal processing windows.

e. Alloy Design and Reverse Optimization: Setting target properties to inversely deduce suitable alloy compositions, accelerating the development of new high-performance aluminum alloys.

Despite the great potential of ML, challenges remain, including insufficient data quantity and quality, lack of physical interpretability in some "black-box" models, and limited model generalization to different alloy systems or experimental conditions.

5. Conclusion

As materials science moves toward greater efficiency, precision, and mechanism-driven research, the integration of molecular dynamics (MD) simulations and machine learning (ML) technologies is becoming a crucial trend in advancing material design and performance prediction. Particularly in the traditional 3xxx series aluminum alloys, facing limitations in mechanical properties, complex corrosion mechanisms, and challenges in microstructure control, traditional experimental methods reveal only partial insights, and struggles remain in exploring high-dimensional parameter spaces, screening new compositions, and achieving multiscale modeling.

However, this study has not deeply explored multiscale modeling approaches (such as coupling atomic simulations with macroscopic finite element models), nor has it systematically analyzed the potential of emerging ML methods like graph neural networks and reinforcement learning. Future research should further expand the integration of multiscale methods and incorporate cutting-edge intelligent algorithms to accelerate the intelligent design and performance prediction of 3xxx series aluminum alloys.

By using MD simulation data as input or training datasets for ML models, future advancements are expected in the following areas: a. Capturing atomic behavior evolution patterns difficult to express explicitly in MD simulations. b. Mitigating the issue of scarce MD data through deep learning and self-supervised learning techniques. c. Bridging atomic-scale simulations with macroscopic experiments or finite element modeling to achieve truly multiscale material design. d. Utilizing Bayesian optimization strategies to identify optimal compositions and processing windows for high-performance 3xxx series aluminum alloys.

References

[1] *Davis, J. R. (Ed.). (1993). Aluminum and Aluminum Alloys. ASM International.*

[2] *Peng, Y., Wang, S. F., Zhang, Y., & Gao, Y. N. (2012). Simulation and application of molecular dynamics in materials science. Advanced Materials Research, 468–471, 234–238.*

[3] *Ramprasad, R., Batra, R., Pilania, G., Mannodi-Kanakkithodi, A., & Kim, C. (2017). Machine learning in materials informatics: recent applications and prospects. npj Computational Materials, 3, 54.*

[4] *Zhang, H., Liu, X., Chen, W., & Li, Y. (2022). Effects of microstructure, texture evolution and strengthening mechanisms on mechanical properties of 3003 aluminum alloy during cryogenic rolling. Materials Science and Engineering: A, 844, 143150.*

[5] *Zamin, M. (1981). The role of Mn in the corrosion behavior of Al-Mn alloys. Corrosion, 37(11), 627–631.*

[6] *Kao, P. W. (1985). Texture and earing behaviour of cold-rolled aluminium alloy 3004. Materials Science and Engineering, 75, 157–165.*

[7] *Kuksin, A. Y., Stegailov, V. V., & Yanilkin, A. V. (2008). Molecular-dynamics simulation of edge-dislocation dynamics in aluminum. Doklady Physics, 53(5), 261–264.*

[8] *Sundar, A., Chen, G., & Qi, L. (2021). Substitutional adsorptions of chloride at grain boundary sites on hydroxylated alumina surfaces initialize localized corrosion. npj Materials Degradation, 5, 18.]*

[9] *Wang, Y., Freiberg, D., Huo, Y., Zhu, W., Williams, R., Li, M., & Wang, Y. (2023). Shapes of nano Al_6Mn precipitates in Mn-containing Al-alloys. Acta Materialia, 253, 118819.*

DOI: 10.54254/2753-8818/2025.GL24106

[10] *Jha, D., Ward, L., Paul, A., Liao, W., Choudhary, A., Wolverton, C., & Agrawal, A. (2018). ElemNet: Deep learning the chemistry of materials from only elemental composition. Scientific Reports, 8(1), 17593.*

[11] *Coelho, L. B., Zhang, D., Van Ingelgem, Y., De Waele, W., Verbeken, K., & Tuytens, F. (2022). Reviewing machine learning of corrosion prediction in a data-oriented perspective. npj Materials Degradation, 6(1), 32.*