Grain Boundary Motion in Magnetic-Pulse-Welded Al-Fe Bimetal Systems: An Atomistic Simulation Study

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Abstract

Magnetic pulse welding (MPW) is an effective solid-state welding method of joining dissimilar metals such as Al/Steel, Al/Ti, Al/Cu et al. In order to understand fully such important phenomena as atomic diffusion, grain boundary motion, interfacial non-equilibrium-phase nucleation and growth in MPW, a detailed microscopic description of the MPW interface is necessary. This study is an extension of our previous work. In the present work, we extend the simulation investigation to polycrystal aluminium and iron systems using Molecular dynamic (MD) method. The polycrystal systems allow for the study of interfacial segregation. Our simulations present structural information on the GBs in nanocrystalline microstructures. Flat GBs can move when subjected dynamic load resulting from the high-velocity impact. Plots of the ratio of GB atoms versus time show a distinctly different GB migration behaviors between loading and unloading conditions. By contrast with our earlier simulations, it was observed that crystal order and stability are highly preserved in the loading stage. The transformation of grain boundary structural change is due to stress-driven GB migration and temperature dependent as well. Grain rotation mechanism was identified. This work could provide atomistic insights into the grain refinement during MPW process.

Keywords

Magnetic pulse welding, Molecular dynamics, Grain boundaries, Grain rotation

1 Introduction

Magnetic pulse welding (MPW) is a solid state impact welding process, which produces metallurgical bond by high-speed impact between two dissimilar materials (Psyk et al., 2011, Su et al., 2025). The ultrafine-grained structure on the MPW interface was commonly observed, which is regarded as the most essential interfacial property for high-strength joints (Zhang et al, 2022). Zhang et al. (2010) studied the Al-6061/Al-6061 and Cu-110 /Cu-110 interfaces formed by MPW. They reported a grain size of about 50 nm at the interface in the case of Al-6061/Al-6061 and nano-scale lamellar structures in the case of Cu-110/Cu-110. The authors concluded that the refinement of the interfacial structure is due to the rapid and severe plastic deformation at high strain rates. Zhu et al. (2023) observed that grain refinement occurs at the interface of 1050 Al and AZ31 Mg, which is regarded as a main reason for the excellent performance of the Al/Mg MPW joint. Raoelison et al. (2024) reported a hierarchical nano-featured structure is confined within a very short total distance of about 200 nm at the Al/Cu interface during magnetic pulse impact welding. Outside these confined nanostructures, the interface exhibits a crystalline structure. Although a large volume of experimental data on the grain refinement generated by the magnetic pulse welding (MPW) process has been accumulated over the recent years, the above experimental research is not sufficient to understand its micro mechanism systematically.

Molecular dynamic (MD) simulations, on the other hand, can give real-time microstructure evolution with atomic-level details (Rapaport et al., 1996). Such atomistic simulations generate temporal-spatial information on three-dimensional atomic configurations and atom trajectories, which can be analysed to gain scientific insights into a physical system.

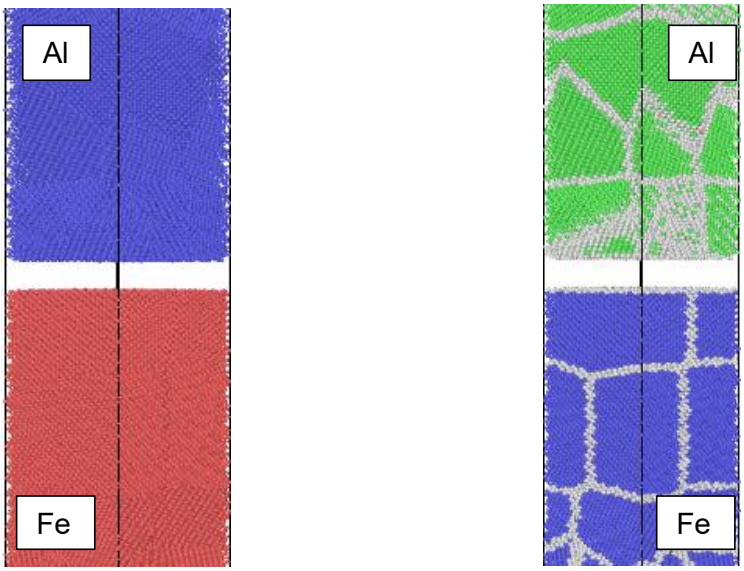
In this paper, we present the details of atomic motion and structural evolution across the interfacial zone for a Fe-Al system in the MPW process. Our goal is to provided illuminating insight into the atomic scale processes that occur during the MPW process.

2 Model and simulation methods

The open-source code, namely Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package, was used to perform the large-scale molecular dynamics(MD) simulations. Three dimensional nanocrystalline Al-Fe samples with mean grain size of 5.5 nm have been constructed by a computer code. The selection of a mean grain size of 5.5 nm was primarily driven by its relevance to experimentally observed nanocrystalline structures and the critical need to capture essential grain boundary (GB) phenomena within computationally feasible limits. This specific size represents a deliberate balance between achieving physical representativeness and managing the substantial computational demands inherent in large-scale MD simulations. Grain orientations were randomly arranged in the samples. Fig. 1 presents the atomic configuration of the initialisation of the developed MD models, in which two metal bulks,

Al (84530 atoms) and Fe (116602 atoms) were put inside a simulation box with dimensions of 10 (X) × 10 (Y) × 48 (Z) nm^3. Between them, vacuum is used to isolate the bulks' initial free surfaces. Periodic boundary conditions have been applied in the two transverse directions (x and y directions) .

A constant integration time step of 1 fs was used for all simulations in this study. Simulation procedure is as follows. In the beginning process, Nose-Hoover thermostat was adopted and the whole system was relaxed at corresponding temperatures and 1 standard atmospheric pressure as an ambient pressure under the constant-pressure-temperature (NPT) ensemble to finish the initialisation. The initial thermal velocities of atoms were assumed to follow a Gaussian distribution. Subsequently, the Al bulk was given a velocity to simulate the collision. The system was relaxed for 1000 ps under the microcanonical (NVE) ensemble. In the end, with the final equilibrium temperature of the NVE simulation kept, the system was relaxed for another 1000 ps still at 1 standard atmospheric pressure (NPT ensemble). The 1000 ps relaxation period was explicitly chosen to achieve a sufficient duration for the system to establish thermodynamic equilibrium and dissipate any residual artificial stresses or energetic instabilities introduced during the initial setup. This deliberate equilibration step ensures that subsequent simulation data is collected from a stable, representative state of the system.



(a)atom type *(b)common neighbor analysis*

***Figure 1**: Initial configuration of the polycrystalline Al-Fe bimetal systems. (a) atom type identity and (b) common neighbor analysis showing grain boundaries.*

The collisions with transverse velocity were simulated, which is consistent with the experimental study focusing on magnetic pulse welding. The axial velocity uz was set at 450 m/s and the transverse velocity ux was set at 250 m/s. The impact velocity applied in the Molecular Dynamics (MD) model is derived from the impact velocity information obtained through Finite Element Analysis (FEA) (Fan et al., 2016). Furthermore, the FEA

model itself is constructed under conditions identical to those of the Magnetic Pulse Welding (MPW) experiments. This consistency ensures that the velocity boundary conditions implemented in the MD simulations accurately reflect the dynamic loading boundary inherent in the MPW process.

An embedded-atom method (EAM) potential for Al-Fe bimetal systems was used in the simulations. The visualization of the atomic configurations was performed by the Open Visualization Tool (OVITO) software (Stukowski, 2009).

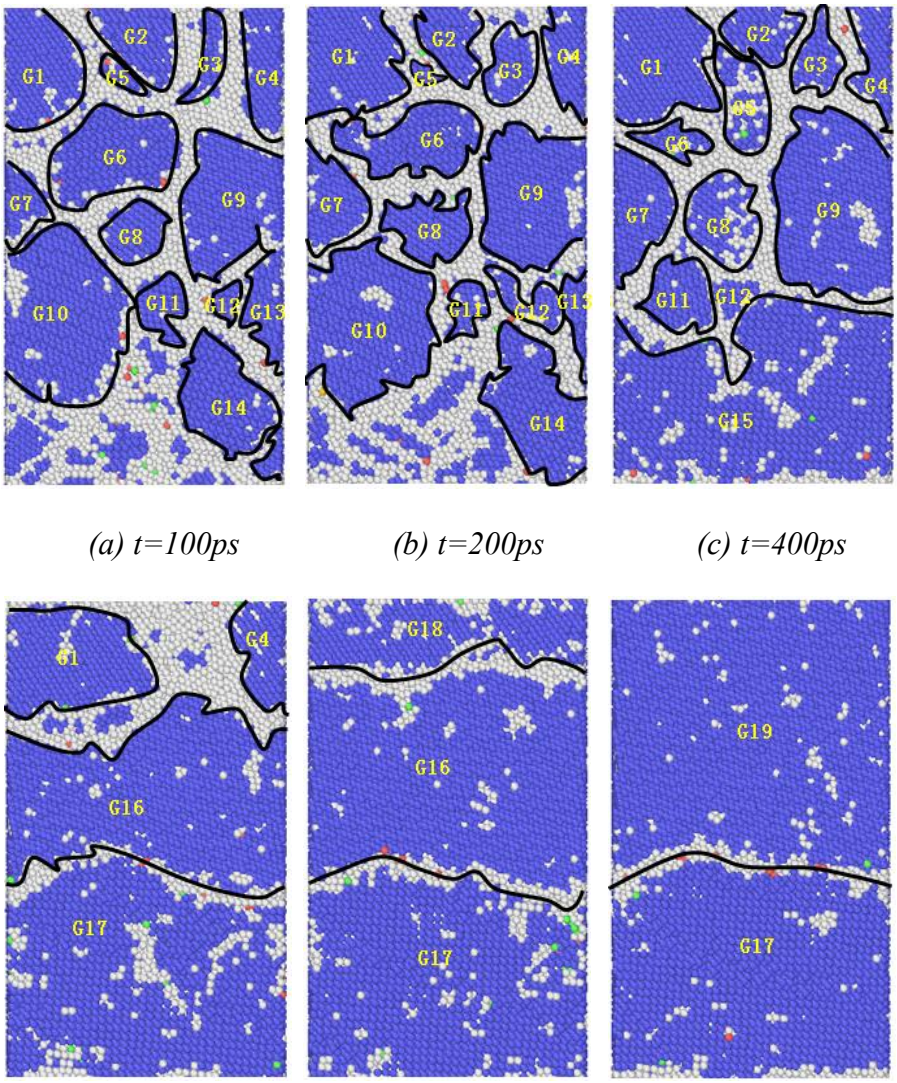
3 Results and discussion

To provide a more intuitive explanation of grain boundary (GB) deformation during the collision process, several grains in the Fe-side matrix from Figure 1(b) were numbered.

Figures 2(a)-(f) display the grain configurations of the Fe-side matrix at different time during the NVE ensemble simulation phase. From (a) to (c), the GB between G1 and G2 gradually thinned. The G1 grew larger and larger by incorporating surrounding disordered GB atoms, while the G2 shrank and became more prone to merging with adjacent larger grains. At t=400 ps, the shrinkage of G6 could be clearly seen through GB migration as G7, G8, and G9 absorbed nearby atoms. Concurrently, G12 and G13 gradually disappeared and merged with GBs of G10 and smaller grains below, ultimately forming a new grain G15. By t=600 ps (Figure 2(d)), G1 further expanded, and the GBs among G7, G8, and G9 merged to form a larger grain G16, while G11 was fully consumed by its adjacent larger grain G15. Due to the higher kinetic energy of atoms at GBs between small and large grains (Zhou, et al., 2014), these GBs exhibit enhanced atomic mobility and are more prone to migration.

Figures 2(d)-(f) reveal that disordered atoms gradually occupied lattice positions, causing GBs between grains to thin. For instance, the GB between G1 and G4 thinned and vanished, forming a new grain G18. Similarly, the GB between G16 and G18 disappeared, creating an even larger grain G19. GB migration arises from atomic movements perpendicular to the GB interface, where atoms diffuse from one grain to another, driving grain growth or shrinkage. This process ultimately leads to coarsening of Fe-side matrix grains during the loading stage. Grain boundary migration under shock loading leads to an alignment of grain boundaries perpendicular to the loading direction.

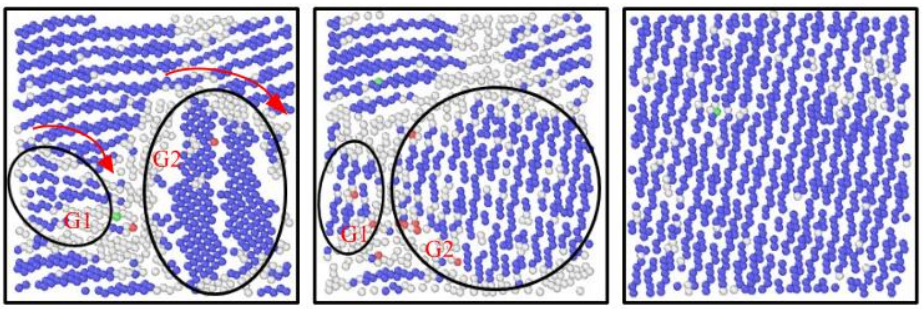
Figures 3 illustrate atomic configurations of a specific layer in the Fe-side matrix at 600 ps, 800 ps, and 1100 ps. Between 600 ps and 800 ps, G1 and G2 rotated clockwise. Under high-speed impact loading during magnetic pulse welding, GB atoms and grain atoms moved in mismatched directions, inducing mutual sliding that drove grain rotation under complex stress conditions.



(a) t=100ps *(b) t=200ps* *(c) t=400ps*

(d) t=100ps *(e) t=200ps* *(f) t=400ps*

***Figure 2**: Snapshots of grain configurations of the Fe-side matrix at different time during the NVE ensemble simulation phase.*



(a)t=600ps *(b)t=800ps* *(c)t=1100ps*

***Figure 3**: Atomic configuration of a layer of atoms on the Fe-side matrix at different times during the NVE ensemble simulation phase. The red arrow indicates the clockwise direction of rotation of the grain.*

To further clarify GB evolution during Al/Fe magnetic pulse welding, statistical analyses of GB atom ratios in the matrix-side regions were performed. Figure 4 shows temporal variations in GB atom proportions across different zones. During the NVE ensemble mechanical relaxation phase, GB atom ratios in both Al- and Fe-side matrices progressively decreased, indicating that under high-pressure impact, fragmented grains reformed into coarser grains. Conversely, during the NPT ensemble thermal relaxation phase, GB atom ratios gradually increased and stabilized. This result shows that as pressure releases, the atomic activities around the GB were more intense at the high temperature, which led to an increase of average thickness of GB. Therefore, the movement of GB became the main factor that affected the microstructure of the Fe-side matrix.

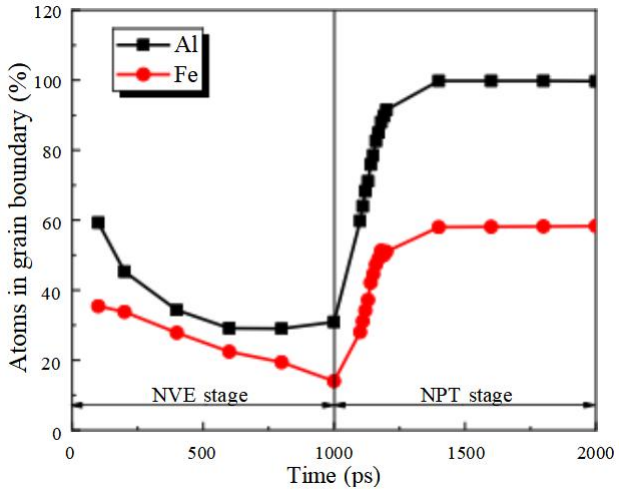
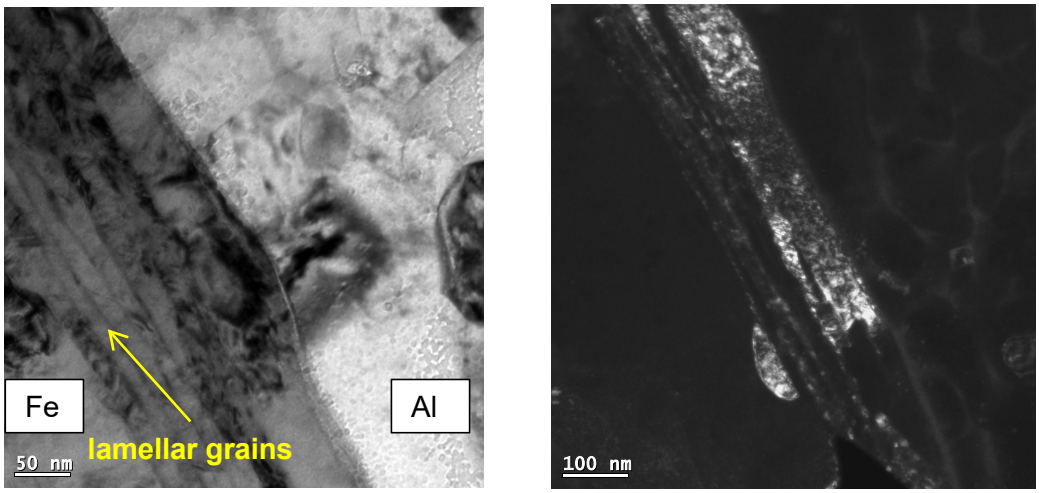


***Figure 4**: The fraction of atoms in grain boundary as a function of time.*

Figure 5 shows bright-field (BF) and dark-field (DF) transmission electron microscopy (TEM) images of the Fe-side matrix microstructure adjacent to the Al/Fe welding interface. The BF image in Figure 5(a) reveals a lamellar grain structure in the Fe matrix. Fe grains directly adjacent to the Al/Fe interface exhibit nanoscale elongated morphologies, while slightly farther from the interface, the Fe grains on the steel side display stacked elongated configurations. These TEM experimental observations of grain morphology are consistent with the MD simulation results.



(a)BF *(b)DF*

***Figure 5**: Transmission electron microscopy (TEM) images of the Al/Fe welding interface. (a) bright-field (BF);(b) dark-field (DF).*

4 Conclusion

Due to the extreme difficulty of constructing and interpreting experiments on atomic-scale level, computer simulation has become an important tool, not only in its usual role of aiding in the development and evaluation of interface theories, but also in determining the basic microscopic phenomenology of crystal/ crystal interfaces. In the current work, the dynamic microstructure evolution and atomic motion in a magnetic-pulse-welded Al-Fe bimetal system have been investigated using the MD method. The key findings are summarized as follows:

(1) Under impact loading, grain boundary (GB) atoms exhibit significant diffusion across adjacent grains, resulting in either grain growth or shrinkage. The deformation process is primarily governed by GB sliding accompanied by rotation of smaller grains.
(2) Impact-induced grain boundary migration causes preferential alignment of GBs perpendicular to the loading direction, suggesting a stress-driven reorganization of the microstructure.
(3) The MD-predicted lamellar nanocrystalline structure in the iron matrix shows good agreement with transmission electron microscopy (TEM) observations, validating the simulation approach.

These simulations provide atomic-level insights into the structural transformations and unique mechanical properties of MPW joints, bridging the gap between theoretical predictions and experimental observations. The findings contribute to a fundamental understanding of interface formation mechanisms in high-speed solid-state welding processes.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (Grant No. 51705081), Natural Science Foundation of Fujian Province of China (Grant No. 2022J01070), and Fuzhou University Testing Fund of precious apparatus (Grant No.2024T018).

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