Molecular Dynamics Modeling of Atomic Diffusion Across Fe-Al Magnetic-pulse-welding Interface

Zhisong Fan[1], Haiping Yu[2*], Jianghua Deng[1], Chunfeng Li[2]

[1] School of Mechanical Engineering and Automation, Fuzhou University, China;
[2] National Key Laboratory for Precision Hot Processing of Metals, Harbin Institute of Technology, China
*Corresponding author. Email: haipingy@hit.edu.cn; Tel: +86-451-86413970

Abstract

In the present study, a molecular dynamic model has been developed for simulating of atomic diffusion behaviour in the Al-Fe system during the magnetic pulse welding process. Our simulations predict the structural evolution of the interfacial region. And the thickness of diffusion layer was studied. The atomic diffusion features at the bonding interface were investigated in detail. Furthermore, the concentration distribution of the elements across the diffusion layer was also presented in this paper. To verify the simulation results, relevant verification experiments were also carried out. The simulation results show a good correspondence with the experiments.

Keywords

Magnetic pulse welding, Atomic diffusion, Molecular dynamics, Interface

1 Introduction

Magnetic pulse welding(MPW) is well known for its capability to directly join a wide variety of both similar and dissimilar metals that can hardly be joined by traditional welding techniques (Psyk et al., 2011, Kapil et al., 2015). Whilst the MPW process is generally successful, the understanding of its physical process and mechanism is far more satisfactory. Particularly, diffusion, one of the important physical phenomena for the formation of the MPW joints, is accelerated under the extreme conditions during the MPW process. In literatures, there have been numerous experimental diffusion studies via energy dispersive spectroscopy (EDS) microanalysis. Akbari Mousavi and Sartangi (2009) used

energy dispersive spectroscopy (EDS) microanalysis and obtained the concentration distributions after the diffusion across the interface between the explosively welded cp-titanium/AISI 304 stainless steel composites. Hokamoto et al. (2009) measured and analysed the elemental distribution after the diffusion across the interfacial zone for metallic glass and stainless steel. Yu et al. (2013) conducted MPW experiments on steel-Al tubular members. The weld interface was subjected to mutual diffusion of Fe and Al elements. Zhang et al. (2011) investigated the chemical composition changes cross the interface by EDS from different locations. The composition gradually changes from one phase to other phase with several steps at the interface with intermetallics. However, experimental approach to the nanoscale system still has a limit to interpret the reaction phenomena originated from the atomistic level.

Molecular dynamics (MD) simulation is nowadays standard methods for materials modeling with atomic scale resolution (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 fully dynamic atomistic simulations of diffusion across the interfacial zone for a Fe-Al system in the MPW process. Our goal is to study the diffusion behaviour and to understand what happens to the MPW interfacial zone under the MPW conditions.

2 Model and simulation methods

In our simulations, 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. Fig. 1 presents the configuration of the initialisation of the developed MD models, in which two metal bulks, Al (6958 atoms) and Fe (10100 atoms) were put inside a simulation box with dimensions of 2.835 (X) × 2.835 (Y) × 30.7 (Z) nm^3. The contact surfaces of Fe and Al are both (0 0 1) planes. 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) which can extend the proposed MD model to simulate the infinite system while for z direction, the large scale was used to make the atoms adequately move.

Molecular dynamics simulation consists of the numerical, step by step, solution of the classical equations of motion. The Newton's equation of motion for the atoms is numerically integrated using the leap-frog algorithm (Plimpton, 1995). 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 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 550 m/s and the transverse velocity ux was set at 250 m/s.

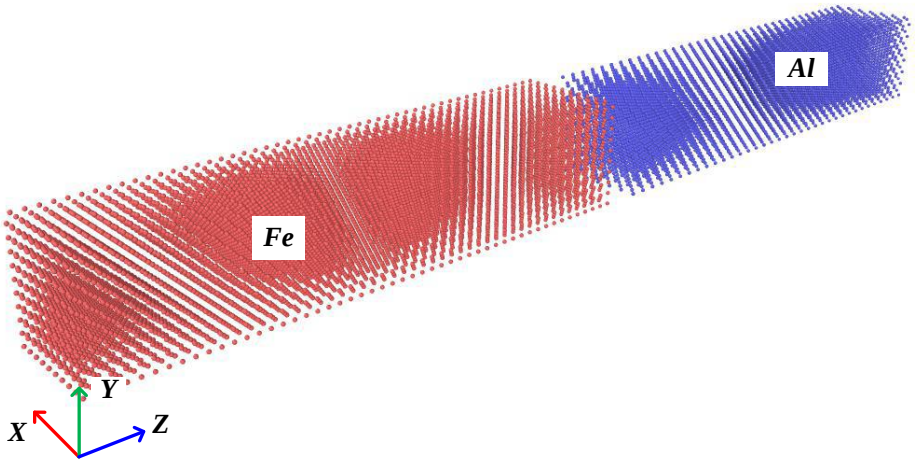


***Figure 1**: MD model of Fe-Al system at the initial state*

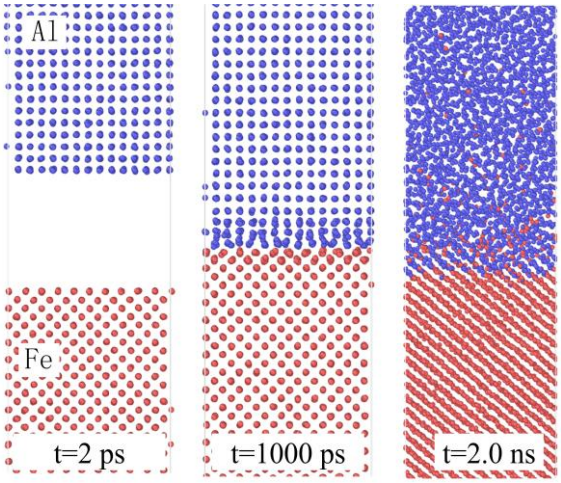
Interatomic potentials play a very important role in MD simulations. Considerable progress has been made in the development of empirical and semi-empirical many-body potentials. Well-established embedded atomic method (EAM) potentials (Finnis and Sinclair, 1984) have been successfully used in analysing elastic properties, defect formation energy and fracture mechanisms of various close-packed bulk metals. Therefore, interaction among iron and aluminium atoms was modelled with the EAM interatomic potential.

The diffusion process was viewed and recorded using the visualization software OVITO (Stukowski, 2009).

3 Results and discussion

Fig. 2 shows the initial setups for the Fe-Al bimetallic system (see Fig. 2a) and the evolution of the atomic structure of the MD model during the collision process of MPW. As illustrated in snapshots of molecular configurations in Fig. 2(b), the contact interface between Fe (bottom, red) and Al (top, blue) is relatively smooth (t = 1 ns). There is no obvious structural change since both sides retain their initial lattice structures. As the inter-diffusion proceeds (see Fig. 2c), the iron atoms penetrate the Al matrix, while at the same time, a portion of Al atoms also diffuse into Fe matrix. It is also observed that inter-diffusion presents asymmetric characteristic, i.e., the Fe atoms diffuse deeper into Al side than the Al atoms into Fe side. This is because Fe atoms have a smaller radius (1.241Å) than that of Al atoms (2.886 Å). Obviously, it is easier for smaller atoms to diffuse into a region of larger atoms. On the other hand, the melting point of Fe is higher than that of Al,

making it harder to break the bonds between Fe atoms than those between Al atoms, making it more difficult for Al atoms to diffuse into the Fe lattice. What's more, the bonds in Al are weaker and vacancies form more easily. All three factors favour the diffusion of Fe atoms into Al, and not the other way around.



(a) t=2 ps (b) t=1000 ps (c) t=2000 ps

***Figure 2**: MD simulation snapshots for Fe-Al bimetallic system at (a) 2 ps, (b) 1000 ps and (c) 2000 ps (The red balls represent Fe atoms and blue balls refer to Al atoms)*

Fig. 3 shows the configuration of a cross-section of the structure after 2000 ps of diffusion at velocity of 650m/s. As can be seen, more Al atoms have diffused into the Fe side. When increasing the collision velocity further (i.e., above 650m/s), the temperature of the Fe-Al system increases. When the temperature exceeds the melting points of Fe, more significant diffusion of Al atoms into Fe is seen, forming an inter-diffusion interfacial region.

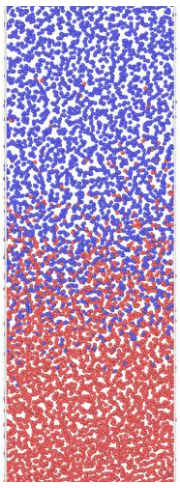
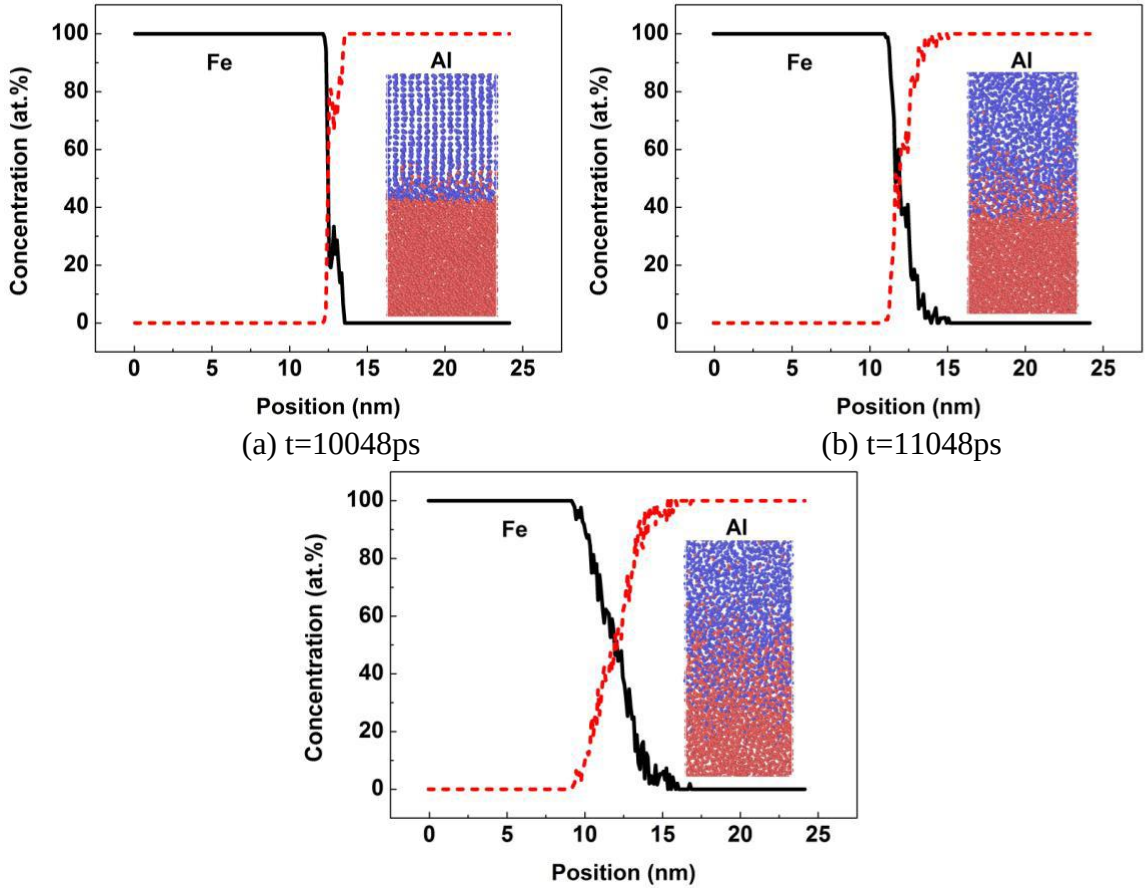


***Figure 3**: The cross-section of the system obtained under temperature over the melting point of Fe*

Fig. 4 shows the concentrations of Fe and Al atoms along the vertical direction for the case in Fig. 3. The region spanning both sides of the interface where the concentration of the solute atoms is over 5% is defined as the interfacial region. The size of this region can be determined from the concentration profiles. At 10048 ps, the thickness is approximately 3 Å (Fig. 4a), indicating very little diffusion across the interface. The thickness increases as the time goes on.



(a) t=10048ps (b) t=11048ps

(c) t=12048ps

***Figure 4**: Concentrations of Fe and Al atoms along the vertical direction at time of (a)10048 ps, (b) 11048 ps and (c) 12048 ps.*

Fig. 5 shows the thickness of the interfacial region as a function of time. As can be seen, the thickness of diffusion layer basically has a linear correlation with the root of diffusion time. In experiments, the diffusion time can be considered to be in the range 1 μs~10 μs. Due to constraints on the time scale, MD simulations cannot capture the evolution of the system for so long time. However, we have good reasons to extrapolate the duration of the diffusion with a constant diffusion coefficient. So, though our MD simulations for 2000 ps, we attain that the diffusion layer thickness is in the range from 1.11 μm (1 μs) to 2.78 μm (6 μs).

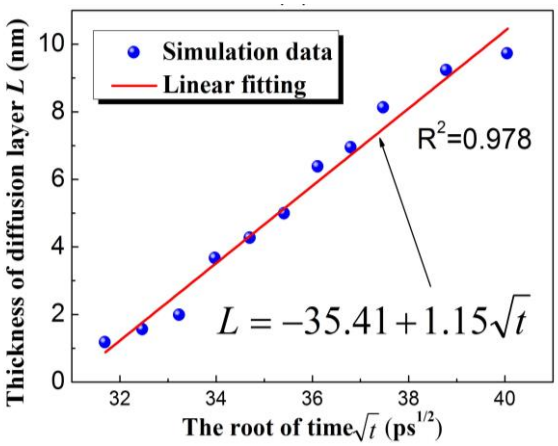


***Figure 5**: Thickness of the interfacial region as a function of time*

Fig. 6 shows the concentrations of Fe and Al atoms across the interfacial region via by Energy-dispersive-spectrometer(EDS) line scanning. Image inserted in Fig. 6 depicts the interfacial microstructure of the Al/Fe bimetallic sample obtained using MPW, which is free of defects like cracks. The scanning lines are across the bonding interface and the diffusion layer. The curves represent the percentage of the atom number at positions along the scanning line. As shown in Fig. 6, the percentages of the number of Fe atoms between the dash vertical lines are 5% and 90% respectively, and they can be roughly considered as the critical points between the diffusion layer and the non-diffusion area. Thus, the thickness of the diffusion layer is about 2.65 μm. The MD simulation results are basically in accordance with the EDS experimental results.

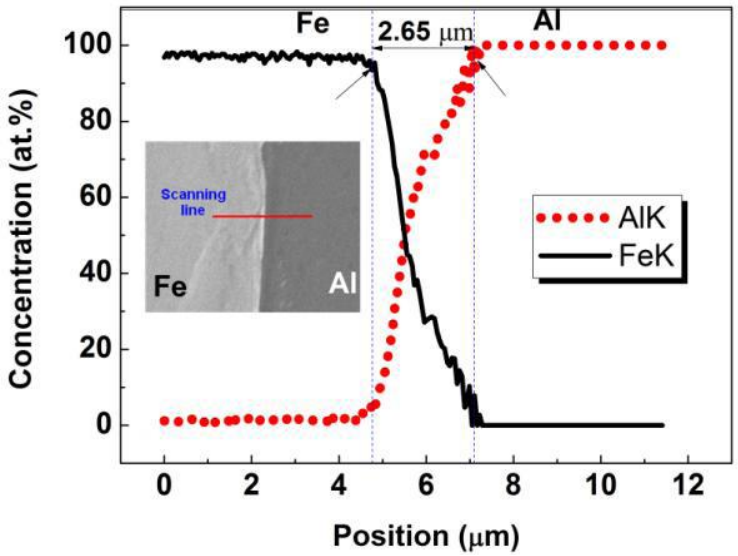


***Figure 6**: Concentration distribution across the interfacial layer of the Fe/Al bi-metallic sample fabricated by MPW*

4 Conclusions

Using MD simulations, we studied the atomic diffusion behaviour in the Al-Fe system during the magnetic pulse welding process. The following conclusions can be drawn.

- As a result of the difference between the melting points of Fe and Al, inter-diffusion presents asymmetric characteristic.
- Fe atoms diffuse more easily into the Al side, while Al atoms largely diffuse into the Fe side only under relatively high collision velocity.
- Calculation of the thickness of the diffusion layer is basically in accordance with the EDS experimental result, which indicates that the developed MD model in present study is valid to investigate the diffusion phenomena.

Simulations of the kind reported here offer an opportunity to examine and understand the fundamental atomistic mechanisms that underlie magnetic pulse welding and can provide ideas for improvement quality of the MPW joints

Acknowledgments

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References

Finnis, M. W., Sinclair, J. E., 1984. A simple empirical N-body potential for transition metals. Philosophical Magazine A, 50(1): 45-55.

Hokamoto, K., Nakata, K., Mori, A., Tsuda, S., Tsumura, T., Inoue, A., 2009. Dissimilar material welding of rapidly solidified foil and stainless steel plate using underwater explosive welding technique. Journal of Alloys and Compounds, 472(1), 507-511.

Kapil, A., Sharma, A., 2015. Magnetic pulse welding: an efficient and environmentally friendly multi-material joining technique. Journal of Cleaner Production, 100, 35-58.

Mousavi, S. A., Sartangi, P. F., 2009. Experimental investigation of explosive welding of cp-titanium/AISI 304 stainless steel. Materials & Design, 30(3), 459-468.

Psyk, V., Risch, D., Kinsey, B.L., Tekkaya, A.E., Kleiner, M., 2011. Electromagnetic forming – A review. Journal of Materials Processing Technology 211 (5), pp. 787-829.

Plimpton, S., 1995. Fast parallel algorithms for short-range molecular dynamics. Academic Press Professional, Inc.

Rapaport, D. C., Blumberg, R. L., McKay, S. R., Christian, W., 1996. The art of molecular dynamics simulation. Computers in Physics, 10(5), 456-456.

Stukowski, A., 2009. Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool. Modelling and Simulation in Materials Science and Engineering, 18(1), 1-7.

Yu, H., Xu, Z., Fan, Z., Zhao, Z., Li, C., 2013. Mechanical property and microstructure of aluminum alloy-steel tubes joint by magnetic pulse welding. Materials Science and Engineering: A, 561, 259-265.

Zhang, Y., Babu, S. S., Prothe, C., Blakely, M., Kwasegroch, J., LaHa, M., Daehn, G. S., 2011. Application of high velocity impact welding at varied different length scales. Journal of Materials Processing Technology, 211(5), 944-952.