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Atomic diffusion behavior and diffusion mechanism in Fe–Cu bimetal casting process studied by molecular dynamics simulation and experiment

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Abstract

A molecular dynamics (MD) method with an embedded atomic method (EAM) was proposed to study the atomic diffusion behavior and diffusion mechanism in the Fe–Cu bimetal casting process. The results indicated that the diffusion coefficient of the Cu atoms was larger than that of the Fe atoms at the same temperature, but the Fe atoms predominantly diffused into the Cu side in the process of diffusion bonding. Moreover, the relationship between diffusion distance and temperature was predicted by the established model, and the optimal temperature for interface diffusion bonding of Fe–Cu bimetal ranged from 1473K to 1753 K. The diffusion behavior was mainly due to vacancies, which played a key role in the formation of the Cu cluster, and the accumulation of Cu atoms decreased the system energy. Finally, Fe/Cu bimetal casting was prepared to validate the simulated results of the diffusion behavior and diffusion distance, and the simulated results were consistent with the experimental ones.

1. Introduction

Bimetal casting has been widely applied in industrial production for a few decades [1–3]. Combining the unique and numerous advantages of two metals is important to improve the properties of a bimetal, such as a copper and ferrite compound structure formed by a bimetal casting process. However, controlling the diffusion bonding and the diffusion layer thickness plays a critical role in bimetal casting technology [4]. A few studies on the atomic diffusion of the Fe/Cu interface in the bimetal casting processes have been carried out by simulation [5–7]. Jelena et al [5] investigated a copper model for continuous steel casting by using a thermo–mechanical analysis. Several material models and service lives were studied and compared, and the results indicated the combined nonlinear kinematic and isotropic material model required huge computational time to reach a stabilized stress–strain loop. Stepanova et al [7] studied the structural change in the cast hypoeutectoid steel with an increase of the copper amount, and a gradual refinement of ferrite grains and pearlite components was obtained with an increase of copper amount. However, for these studies mentioned above, the diffusion mechanism has rarely been reported, particularly the diffusion behavior of the Fe/Cu interface. In addition, it has been reported that the diffusion bonding of bimetal casting and the interface layer is temperature-dependent [8–10], while the preheating temperature of the steel matrix is completely dependent on empirical data at present, in particular, the solid diffusion temperature of a bimetal reaches 0.5–0.8 T_m (T_m is the lower melting point of the two metals) [9–11]. Moreover, the solid–liquid diffusion temperature of the Fe–Cu bimetal has rarely been studied.

MD simulation are advantageous in revealing the atomic–scale structure evolution and interpreting the relevant experiments at the microscopic scale [12]. The simulation of the Al–Cu interface diffusion in an explosive welding process[13, 14] illustrated that the most suitable temperature of diffusion bonding was 750 – 800 K, and the diffusion layer thickness was 5 – 10 μm. Zhu et al [15] studied the interface diffusion
between metallic glass CuZr crystals at the atomic scale, and found that the intrinsic diffusivity was in the order: Cu > Al > Zr. You [16] illustrated that the aggregation of Cu atoms in the Fe-1.1% Cu-0.9% Ni ternary alloy was a major cause of the decrease in tensile properties and that the existence of vacancies could improve the diffusivity of Cu atoms in Fe matrix, promoting the formation and precipitation of Cu clusters appreciably [17]. Cui et al [18] reported that the droplets of Cu atoms aggregated in the coagulation process of the Fe–Cu alloy for the adsorption of Fe atoms on the edge of the interface. The vacancy clusters produced in the diffusion process of the Ni–Fe–Cr ternary alloys, leading to the emergence of the stacking fault tetrahedra and the presence of Cr atoms accelerated the transformation process [19–21]. However, there is no relationship between the diffusion layer thickness, preheating temperature and time, which is of considerable significance to better understand the atomic diffusion behavior of the solid-liquid interface of bimetal casting.

In the present study, Fe atoms with the bcc lattice were taken as the simulation model and the heterogeneous transformation was ignored to obtain deep insights into the effect of temperature on the interfacial diffusion. An MD simulation was used to investigate the atomic diffusion behavior in the Fe–Cu bimetal casting process and the effects of temperature on the diffusion bonding of Fe–Cu bimetal and diffusion mechanism at the bonding interface were studied at length. Finally, Fe–Cu bimetal casting was prepared to validate the simulated results.

2. Methodology

2.1. Mathematical model

The atomic interaction between Fe and Cu atoms was described with EAM potentials, exploited by Bonny [22], which was suitable for the system involved. In the potential function, the total energy consisted of two parts: one was the interaction potential between the nuclei in the crystal lattice, and the other was the embedded potential generated by all the other atoms except item \( i \), which could be expressed as follows:

\[
\Phi = \sum_i E_i(\rho_i) + \frac{1}{2}\sum_{j\neq i} \Phi_{ij}(r_{ij})
\]  

(1)

Where, \( E_i(\rho_i) \) indicated the embedded potential, \( \Phi_{ij}(r_{ij}) \) denoted the pair potential, and represented the sum of the electron density in place of item \( i \) generated by all the other atoms except item \( i \). Here, \( \rho_i \) could be expressed as follow:

\[
\rho_i = \sum_{j\neq i} \rho_{ij}(r_{ij})
\]  

(2)

The accuracy of the EAM potential was confirmed in previous studies [23–25], and the potential function coincided with that of the present study.

2.2. Simulation method

MD simulations of the bimetal casting process in this work were carried out with the LAMMPS package [26]. The simulated box contained two separated metal bulks, namely bcc-Fe atoms and fcc-Cu atoms. Periodic boundary conditions were applied along the x and y axes. The contact surface between the two bulks was an ideal (001) plane and that of the two separated metal bulk was \( 12 \times 6 \times 60 a_{Cu}^\text{Fe} = 10 \times 5 \times 60 a_{Cu}^\text{Cu} \) (aFe = 0.28664 nm, aCu = 0.36147 nm), respectively, while the position of the bottom five layers, as well as that of the top layer, were fixed so that the cubic system could be viewed as a semi-infinite wide interface coupling, as shown in figure 1. In this study, the constant-pressure-temperature (npt) ensemble was used, and the time step was set to 2 fs. Meanwhile, the initial velocity of the atoms was assumed to be consistent with the Maxwell-Boltzmann random distribution and the Verlet integration algorithm was introduced to solve the Newtonian equation of motion integration.

The system was optimized statically with a conjugate gradient (CG) algorithm to complete the energy minimization. Considering that the diffusion temperature of Cu and Fe atoms is above the melting point of Cu (Cu: 1356 K and Fe: 1811 K) in the Fe–Cu bimetal casting process, the box was heated from 300 K to the target
temperature (1373 K, 1423 K, 1473 K, 1523 K and 1573 K, respectively) in 200 ps. Note that only when the temperature range was 0.6 ~ 0.8 Tm (Tm denotes melting point), atoms on either sides of the interface could diffuse into the opposite side significantly [27]. Then, the box was equilibrated adequately for 2000 ps at the corresponding temperature, and the atomic diffusion occurred during this period. For the next 1000 ps, the thermal result was continuously output by the open visualization tool (OVITO) used for post-processing the data.

2.3. Experimental process

DT4 pure Fe and pure Cu were used to fabricate the Fe–Cu bimetal: pure Fe was taken as a matrix, covered by active agents and then heated to 1473 K. The molten pure Cu was poured into the Fe matrix at 1473 K. The casting process is shown in figure 2.

The macrophotograph of the Fe–Cu bimetal is shown in figure 3(a), and the dimensions are noted in figure 3(b). A sample of dimensions φ50 mm × 10 mm was cut from the middle of the Fe–Cu bimetal casting, as shown in figure 3(b). The sample was abraded with various grades of SiC paper followed by mechanical polishing with a 0.5 μm alumina pastes to a mirror, and rinsed with deionized water, the cleaned sample was shown in figure 3(c). The Fe matrix and the Cu layer of the Fe–Cu bimetal were etched by a 5% nitric alcohol solution and a ferric chloride hydrochloric acid solution, respectively. The interface bonding was observed by scanning electron microscopy (SEM), and the elemental analysis of the interface was performed using x-ray photoelectron spectroscopy. Then, three points were taken from the bimetal (figure 3(b)) for the cooling curve simulation.

3. Results and discussion

According to the theory of mismatch degree, the energy of interface in different directions was calculated, and then Fe (100) and Cu (100) were selected after optimization analysis. The interface was set up by 6a × 6a × 6a Fe block and 6a × 6a × 6a Cu block, and the positions of Cu and Fe atoms in 55 layers near the interface were tracked and recorded. The relationship between the interface energy and interface spacing was established as shown in figure 4. It can be seen that the system energy is the minimum when the interface spacing is 1.6 Å, resulting in the strongest adsorption work and the most stable interface structure. Besides, the function of mean square displacement of Cu and Fe atoms were obtained, and the diffusion behavior would be analyzed based on the data.

3.1. Mutual diffusion between Fe and Cu

Figure 5 presents the configurations of the (001) plane at different temperatures at 3.6 ns. A red ball represents an Fe atom and a blue ball denotes a Cu atom, and the initial distance of the interface in figure 5(a) is 1.6 Å. It can be seen that the Fe atoms transferred deeply into the Cu side across the interface, but only a few of Cu atoms were incorporated into Fe side and the diffusion distance was relatively short. The interface thickness increased as the temperature increased from 1373 K to 1573 K, suggesting that the mutual diffusion process was temperature-dependent. The atomic thermal movement with a greater average of molecular kinetic energy increased with an increase of temperature, which led to significant diffusion and increased interface thickness. As the temperature was higher than the melting point of Cu and lower than that of Fe, the inter-atomic force in the Fe atoms was stronger than the bonds among the Cu atoms, which was beneficial for the diffusion of the Fe atoms into the Cu side. With an increase of temperature, the diffusion of the Cu atoms increased because of the higher energy obtained to overcome the migration energy barrier.
The mean square displacement (MSD) curves of the Fe and Cu atoms at different temperatures are shown in figure 6. The higher the temperature was, the larger were the MSD values of the Fe and Cu atoms. It can also be seen that the MSD value of the Cu atoms maintained a higher level at all the considered temperatures, while the MSD value of the Fe atoms increased sharply when the temperature increased to 1523 K, implying that the mobility of the Fe atoms had been enhanced substantially. Furthermore, linear trends could be observed from the plotted MSD curves of the Fe and Cu atoms, which provided a direct estimation of the diffusion coefficients.

Figure 3. (a) Fe–Cu bimetal casting, (b) dimension of the bimetal, and (c) cleaned sample for analysis.

Figure 4. Relationship between the interface energy and interface spacing.
According to the Einstein diffusion law [14], there was a certain correlation between the diffusion coefficient and the casting temperature, and the diffusion coefficient $D$ could be expressed as follows:

$$D = \lim_{t \to \infty} \frac{1}{2Nt} \langle |r(t) - r(0)|^2 \rangle$$  \hspace{1cm} (3)

where $t$ denoted time and $N$ represents dimensionality of the system. In the present study, the simulation configuration was undimensional and diffusion occurred only in the direction perpendicular to the interface, therefore, the value of $N$ was taken as 1 and the $D$ was equal to half of the slope of the MSD curve.

The diffusion coefficients of the Fe and Cu atoms at different temperatures are shown in table 1. It can be seen that the diffusion coefficients of the Fe and Cu atoms increased with an increase of temperature, and the diffusion coefficient of the Fe atom was lower than that of the Cu atom at the same temperature by approximately 44 ~ 470 times. With the increase of temperature, the diffusion coefficient of the Fe atoms increased significantly, and the ratio of $D_{Fe \rightarrow Cu}$ to $D_{Cu \rightarrow Fe}$ varied from 82 to 44 when the temperature increased to 1523 K and 1573 K, respectively.

Using Arrhenius’ equation, the diffusion activation energies of the Fe and Cu atoms were calculated. The calculated diffusion activation energies of Fe and Cu were 209 kJ mol$^{-1}$ and 36 kJ mol$^{-1}$, respectively. Table 2 shows a comparison of the diffusion activation energies of the Fe and Cu atoms reported in previous literatures [20, 28]. Note that the diffusion activation energy calculated in this study was relatively small, and the main reason was that diffusion activation energies reported in previous studies were obtained during a solid-solid diffusion process.
3.2. Prediction of interface diffusion distance

When the atomic concentration is greater than 5\%, the corresponding region is considered the interfacial region \[27\], therefore, the thickness of the interfacial region could be confirmed from the concentration profiles. The concentration distributions of the Fe and Cu atoms along the \(z\)-axis at different temperatures are shown in figure 7. The thickness of the interfacial region is approximately 1.15 nm, 1.31 nm, 1.50 nm, 5.34 nm and 6.76 nm at 1373 K, 1423 K, 1473 K, 1523 K and 1573 K, respectively, as shown in figure 8. Moreover, it can be observed that the diffusion thickness increased with the increase of temperature.

Furthermore, the diffusion layer thickness of the Fe/Cu interface increased significantly when the temperature increased from 1473 K to 1573 K, which was consistent with the results shown in figure 5. Combining the results of table 1 and figure 8, it can be concluded that the appropriate temperature range for the Fe–Cu bimetal casting was 1473 K \(\sim\) 1573 K. However, the higher the temperature was, the greater was the erosion tendency of pure iron. Thus, it was optimal to choose the lower limit of the temperature range simulated as the pouring temperature of the Fe–Cu bimetal casting and the preheating temperature of the Fe matrix.

The atomic diffusion at the interface of the Fe–Cu bimetal casting could be considered unidimensional. For the one-dimensional solid diffusion process, the solution of the diffusion equation could be expressed as follows \[15\]:

\[
c(L, t) = \frac{1}{2}\left[1 - \text{erf}\left(\frac{L}{2\sqrt{Dt}}\right)\right]
\]

(4)

where, \(L\) was the one-dimensional diffusion distance, \(t\) denoted time, and diffusion distance conformed to the Gaussian distribution. Therefore, the diffusion distance of the bimetal was proportional to \(\sqrt{Dt}\), and the diffusion distance \(L\) could be calculated according to the following equation.

\[
L = \sum_{i=\text{Fe,Cu}} k\sqrt{D_i} t
\]

(5)

where, \(D_i\) denoted the diffusion coefficients of the Cu and Fe atoms, \(k\) represented a temperature-dependent constant. The values of \(k\) involved in equation (5) at different temperatures were confirmed by an MD simulation and shown in figure 9, and the relationship between temperature and the value of \(k\) could be described as equation (6).

\[
k = 21.67 - 0.0345T + 1.383 \times 10^{-5}T^2
\]

(6)

The simulated results of the thickness of the diffusion layer with time at 1473 K are shown in figure 10, and \(L\) and \(t\) satisfy equation (7). Similarly, the expressions between \(L\) and \(t\) at different temperatures could be obtained, which are listed in table 3.

\[
L = 0.79\sqrt{t}
\]

(7)

The model established in table 3 was used to predict the interface diffusion distance of the Fe–Cu bimetal at different temperatures. When the temperature was in the range of 1373 K \(\sim\) 1423 K, the diffusion of the Cu atoms to the Fe side was dominant, suggesting that the solid diffusion of the Fe atoms could be neglected in the Fe–Cu bimetal casting process. Furthermore, the interface diffusion of the Fe atoms became obvious, the

Table 1. Diffusion coefficients of Fe and Cu atoms at different temperatures.

| Temperature (K) | \(D_{\text{Fe-Cu}}\) \(10^{-11}\text{ m}^2\text{s}^{-1}\) | \(D_{\text{Cu-Fe}}\) \(10^{-11}\text{ m}^2\text{s}^{-1}\) | \(D_{\text{Cu}}/D_{\text{Fe}}\) |
|----------------|---------------------------------|---------------------------------|----------------|
| 1373           | 0.644                           | 3.031                           | 470            |
| 1423           | 1.227                           | 3.364                           | 274            |
| 1473           | 2.711                           | 3.682                           | 135            |
| 1523           | 4.806                           | 3.948                           | 82             |
| 1573           | 10.084                          | 4.464                           | 44             |

Table 2. Comparison of the diffusion activation energies of Fe and Cu atoms reported in the literatures.

| Element | Master alloy | Diffusion factor \((D_0)/\text{m}^2\text{s}^{-1}\) | Diffusion active energy \((Q)\text{kJ mol}^{-1}\) |
|---------|--------------|---------------------------------|---------------------------------|
| Fe      | Cu           | \(5.9 \times 10^{-4}\)         | 209                             |
|         |              | \(1.4 \times 10^{-4}\)         | 217                             |
| Cu      | Fe           | \(0.65 \times 10^{-7}\)        | 36                              |
|         |              | \(5.2 \times 10^{-7}\)         | 58                              |
diffusion distance increased significantly when the interface temperature increased to 1473 K (0.82 times the melting point of Fe), and the solid diffusion of the Fe atoms had to be considered.

### 3.3. Diffusion mechanisms

As demonstrated above, the Fe atoms migrated deeply into the interior of Cu across the interface, but the diffusion coefficient of the Fe atoms was lower than that of the Cu atoms. Further simulations were required to explain the diffusion mechanism of the Fe–Cu bimetal casting. Three $2 \times 2 \times 2$ supercells were built to assess the influence of the Cu atom aggregation on the system energy, as shown in figure 11, and the ratio of the Fe and Cu atoms was 11/5. The segregation of Cu increased from that shown in figure 11(a) to that shown in figure 11(c). On the basis of the statistical analysis, each dimension on the $x$, $y$, $z$ axes were zoomed by 8 times, and 5632 Fe atoms and 2560 Cu atoms were involved. The calculation method has been described at length in section 2.2.

The minimum energies obtained by the optimized calculation of the structures shown in figure 11 at different temperatures are shown in figure 12. It can be observed that when the Cu atoms aggregated the system lay in the lowest energy state at different temperatures, suggesting that the Cu atoms had the tendency to form clusters in Fe lattice. Besides, the energy of Cu atoms segregation system is lower than that of Cu atoms.
Figure 8. Diffusion layer thickness of Fe/Cu interface at different temperatures simulated for 3.6 ns.

Figure 9. Calculated results of temperature-dependent constant $k$ and the fitted curve of $k$ and $T$.

Figure 10. Simulated results of thickness of diffusion layer with time at 1473 K.
dispersion system at the same temperature. The diffusion energy of the atomic clusters decreases and it was not conducive to the jumping of Cu atoms, blocking the further diffusion of Cu atoms. Therefore, it is difficult for Cu atoms to spread to a long distance on Fe side, although Cu atoms have a stronger diffusion capability.

The radial distribution function (RDF) can be interpreted as the ratio of the area density and the average density, and implies a higher probability of other atoms around the selected atom in the location corresponding to the peaks [29]. Figure 13 shows the RDF of different parts (5 layers of Cu atoms near the interface and in the pure Cu region, respectively). Including the temperature system, the RDF peaks of the Cu atoms in the interface region were smaller than those of the Cu atoms on the pure Cu side, which indicated that the arrangement of the Cu atoms was disordered near the interface. In the interface of the Cu atomic region, the coverage area corresponding to the first peak was narrower, and the first peak of the RDF curves split clearly at 1573 K, which

![Figure 11](image1.png)  
**Figure 11.** Three $2 \times 2 \times 2$ super cells to assess the influence of Cu atom aggregation on the system energy.

![Figure 12](image2.png)  
**Figure 12.** Relationship between system energy and temperature.

| Temperature (K) $\bar{T}_m$ | $L_{Fe-Cu}$ (nm$^2$ ns$^{-1}$) | $L_{Cu-Cu}$ (nm$^2$ ns$^{-1}$) | Fitted equation (nm) | Prediction equation (nm) |
|-----------------------------|-----------------------------|-----------------------------|----------------------|-------------------------|
| 1373 ($0.76\bar{T}_m$)      | 0.00644                     | 3.031                       | $L = 0.606\sqrt{T}$ | $L = \sum_{i=Fe,Cu} 0.332\sqrt{D_i T}$ |
| 1423 ($0.785\bar{T}_m$)    | 0.01227                     | 3.364                       | $L = 0.690\sqrt{T}$ | $L = \sum_{i=Fe,Cu} 0.355\sqrt{D_i T}$ |
| 1473 ($0.82\bar{T}_m$)     | 0.02711                     | 3.682                       | $L = 0.790\sqrt{T}$ | $L = \sum_{i=Fe,Cu} 0.379\sqrt{D_i T}$ |
| 1523 ($0.84\bar{T}_m$)     | 0.04806                     | 3.948                       | $L = 2.814\sqrt{T}$ | $L = \sum_{i=Fe,Cu} 1.175\sqrt{D_i T}$ |
| 1573 ($0.87\bar{T}_m$)     | 0.10084                     | 4.464                       | $L = 3.582\sqrt{T}$ | $L = \sum_{i=Fe,Cu} 1.465\sqrt{D_i T}$ |
provided more evidence for the fact that the Cu atoms tended to aggregate and form clusters in the Fe lattice near the interface, leading to a decrease in its intrinsic diffusivity.

3.4. Validation experiment

According to the results of the MD simulation, the Fe atoms could further diffuse into the interior of the Cu side, but the Cu atoms hardly diffused into the interior of the Fe side. An experiment was carried out to validate these results. Figure 14(a) shows the interface of the Fe–Cu bimetal observed by SEM, and the chemical composition of the bonding interface was analyzed by a line-scan of x-ray photoelectron spectroscopy, as shown in figure 14(b). It revealed that the Fe atoms diffused at a low ratio and could deeply diffuse into the interior of Cu, while the Cu atoms diffused at a high ratio and could hardly diffuse into the interior of Fe. The experimental results were in good agreement with the simulated ones.

The solidification of the Fe–Cu bimetal was so rapid that the temperature of the Fe/Cu interface decreased to a value below the liquidus temperature quickly. The cooling curve of special points A, B and C in the Fe–Cu bimetal marked in figure 3 is shown in figure 15. During the casting experiment, both Fe matrix and molten pure Al were kept 1473 K, and figure 15 showed that the interface temperature was between 1373 K and 1473 K only for 1 ~ 19s. According to the model established in table 3, the interface diffusion distance between 1373 K and
1423 K was 19 ~ 54 μm, and the measured diffusion distance in the validated experiment was approximately 25 μm. The simulated result was basically consistent with the measured one, suggesting that it was feasible to predict the interface diffusion distance of the Fe–Cu bimetal casting with the simulated model.

**Figure 14.** (a) Interface of Fe–Cu bimetal observed by SEM and (b) chemical position of the interface (the preheated temperature of both was 1473 K).

**Figure 15.** Cooling curves of special points in Fe–Cu bimetal marked in figure 3.
4. Conclusions

(1) Based on the calculation results of diffusion coefficient and diffusion distance, the solid-liquid diffusion of Fe/Cu interface was asymmetric, and Fe atoms were easier to diffuse into Cu lattice at the same temperature.

(2) The diffusion distance of Fe atoms into Cu lattice was larger than that of Cu atoms into Fe lattice, though the diffusion coefficient of Cu atoms was larger. The diffusion energy of Cu atoms decreased due to the formation of atomic clusters, hindering the further diffusion of Cu atom into Fe lattice.

(3) The Fe/Cu atom diffusion layer thickness was temperature-dependent, and with the increase of temperature, the diffusion distance of Fu atoms into Cu lattice and Cu atoms into Fe lattice increased gradually. When the temperature reached 1473 K, the diffusion distance of Fe atoms into Cu lattice increased rapidly.

(4) The Fe–Cu bimetal casting was prepared at 1437 K to validate the simulated results about the diffusion behavior and the diffusion distance, and the simulated results were consistent with the experimental ones.

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