Particle simulation of nugget formation process during steel/aluminum alloy dissimilar resistance spot welding and thickness estimation of intermetallic compounds

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ABSTRACT
A steel/aluminum alloy dissimilar resistance spot welding process was simulated by a three-dimensional smoothed particle hydrodynamics method. Furthermore, the time-dependent increase in the intermetallic compound thickness at the joint interface was estimated using the obtained numerical data of temperature history. As a result, the steel sheet started to melt from the center of the sheet in the thickness direction. The convection in the molten aluminum alloy caused by the electromagnetic force promoted the heat transfer at the solid-liquid interface because the temperature gradient becomes steeper. Moreover, the maximum thickness of the intermetallic compound was estimated to be approximately 1 mm. These results support the validity of the computational model developed in this study for simulating the nugget formation process during dissimilar resistance spot welding and estimating the intermetallic compound thickness.

KEYWORDS
Resistance spot welding; dissimilar materials; particle method; simulation; intermetallic compound

1. Introduction
Resistance spot welding is a welding method in which overlapped materials are sandwiched between electrodes and energized while applying pressure to form a molten part (nugget) between the materials to be welded by Joule heating to join the materials. Compared with other welding methods, resistance spot welding is widely used in mass production technology for automobiles, railcars and electrical appliances because of its short welding time and ease of automation. In particular, resistance spot welding is used for 3,000 to 6,000 joints in the assembly of automobile bodies [1]. In recent years, environmental measures and the increasing demand for lighter car bodies due to the electrification of automobiles have made it urgent to establish a technology for resistance spot welding of dissimilar materials between steel and aluminum alloys, which are lightweight metals [2,3]. However, it is known that when steel and aluminum alloys are welded, a layer of brittle intermetallic compound (IMC: Intermetallic compound) is formed at the joint interface, which reduces the strength of the joint [3]. To prevent this, research is being conducted to control the intermetallic compound layer formed at the joint interface in resistance spot welding of steel and aluminum alloys with dissimilar materials.

Takeda et al. [4] performed resistance spot welding of dissimilar materials under several conditions by changing the tip shape of the electrode and the thickness of the aluminum alloy, and investigated the relationship between the interfacial reaction layer and joint strength under each condition. As a result, it was clarified that Fe-Al intermetallic compounds of approximately 1 mm were formed extensively under welding conditions where the electrode diameter was large and the thickness of the aluminum alloy was large. The joint strength was higher when such an intermetallic compound of about 1 mm was formed than in other welding conditions. Miyamoto et al. [5] conducted experiments focusing on the Al-Zn eutectic reaction that occurs when galvanized steel sheet is resistance spot welded to an aluminum alloy. Wan et al. [6] found that the formation of a thin and uniform Fe-Al intermetallic compound...
after joining steel and aluminum alloys by resistance spot welding was possible. The observation of the joint cross section revealed that an intermetallic compound consisting of Fe$_2$Al$_5$ adjacent to the steel and FeAl$_3$ adjacent to the aluminum alloy was formed in the center of the joint interface, and a layer consisting of a mixture of FeAl$_3$ and Al was formed at a distance from the center where the aluminum alloy was not molten. The results of this study are as follows. The thickness distribution of the intermetallic compound layer formed under different welding conditions was predicted based on the temperature histories of the interfaces obtained by simulation. The results show that when the welding time is long, the thickness distribution of the intermetallic compound is bimodal.

On the other hand, studies on the prediction of nugget formation process during resistance spot welding and intermetallic compound growth during resistance spot welding of dissimilar materials have been conducted using numerical simulation. Niho et al. [7] have developed a numerical model that comprehensively evaluates analytical methods for the elasto-plastic contact-current-heat conduction triad that occurs during resistance spot welding. The nugget diameters obtained from the analysis of this model were in good agreement with the experimental nugget diameters of the cut surfaces of the welds.

Wang et al. [2] developed a coupled current-temperature-stress analysis model for resistance spot welding of steel and aluminum alloys using the finite element method. The model predicts the thickness of the intermetallic compound based on the thermal history of the joint interface, and the results are in good agreement with experimental results under the same conditions.

As described above, reports have been made on the control of intermetallic phases in resistance spot welding of dissimilar materials, reporting appropriate welding conditions and estimating the thickness of intermetallic phases based on temperature histories obtained from numerical simulations. However, these studies do not take into account changes in the temperature field due to convective heat transport associated with molten metal flow. The welding current used in resistance spot welding is a large current of several kA or more, which exerts strong electromagnetic forces on the molten metal. Therefore, forced convection is considered to occur inside the nugget even though the welding time is short. Convection transports its own heat energy. When thermal energy is transported simultaneously by convection and conduction, the amount of heat transferred to the molten interface is greater and melting is accelerated compared to when thermal energy is transported only by conduction. The same is true at the interface between different materials, where different temperature histories can be expected during the process. Therefore, in order to more accurately predict the thickness of intermetallic phases, it is necessary to construct a computational model that can simultaneously solve for the flow of molten metal in the material being welded and simulate the nugget formation process, taking into account convective heat transport, in addition to conventional coupled analysis.

In this study, the melting and solidification processes of resistance spot welding of dissimilar materials, i.e. mild steel and aluminum alloys, are modeled by considering convective heat transport using the incompressible SPH (Smoothed Particle Hydrodynamics) method [8,9]. The objective is to obtain the temperature history of the joint interface by simulation using this model, and to estimate the thickness of the intermetallic compound layer from the results.

2. Computational model

2.1. Governing equations

The particle method used as a computation method in this study has been also applied in the welding and joining fields such as weld pool convection phenomena in laser, TIG (Tungsten Inert Gas) and MIG (Metal Inert Gas) welding [10–13], metal transfer phenomena in MIG and flux cored arc welding [14,15], and submerged arc welding phenomena [16], and melting inside nuggets during resistance spot welding [17–21] is considered an effective tool for simulating molten metal flow inside nuggets during resistance spot welding. The Lagrange-type equations of motion for incompressible flows, when discretized based on the SPH discretization method, can be expressed as in Equation (1).
\[
\frac{D \mathbf{u}^a}{Dt} = -\sum_b m_b \left( \frac{P_a}{\rho_a} + \frac{P_b}{\rho_b} \right) \nabla_a W_{ab} + \frac{2d}{\rho_a \sum_b |\mathbf{r}_{ab}|^2} W_{ab} \sum_b \left( \eta_a + \eta_b \right) \left( \overrightarrow{u}_b - \overrightarrow{u}_a \right) W_{ab} + \frac{\mathbf{j}_a \times \mathbf{B}_a}{\rho_a}
\]

\[\text{(1)}\]

\[a, b \text{ denote particles, where } \overrightarrow{u} \text{ is the velocity vector, } t \text{ is the time, } m \text{ is the mass, } P \text{ is the pressure, } \rho \text{ is the density, } W \text{ is the kernel function, } d \text{ is the dimension number, } \mathbf{r} \text{ is the relative position vector, } \eta \text{ is the viscosity coefficient, } \mathbf{j} \text{ is the current density vector and } \mathbf{B} \text{ is the magnetic flux density vector.}\]

In Equation (1), the terms on the right-hand side represent the pressure gradient, viscous force and electromagnetic force. In this study, in order to solve the behavior of molten metal, which is incompressible flow, in large time increments, the density homogenizing algorithm [9] is used.

The temperature of the particle is determined from the energy transport equation given in Equation (2).

\[
\frac{DT_a}{Dt} = \frac{2d}{\rho_a C_a \sum_b |\mathbf{r}_{ab}|^2} W_{ab} \sum_b \frac{K_a + K_b}{2} (T_b - T_a) W_{ab} + \frac{\mathbf{j}_a^2 + R_a |\mathbf{J}_a|^2}{\rho_a C_a V_a}
\]

\[\text{(2)}\]

Where \( T \) is the temperature of the particle, \( C \) is the specific heat, \( \kappa \) is the thermal conductivity, \( \sigma \) is the electrical conductivity, \( R_e \) is the contact electrical resistance, and \( S_{ab}, V_a \) are the cross-sectional area and volume of the particle. The terms on the right-hand side of Equation (2) represent the heat generated by thermal conduction, Joule heating, and contact resistance. The current density is obtained from the following conservation law of current and Ohm’s law.

\[
\nabla \cdot \mathbf{j} = 0 \quad \text{(3)}
\]

\[
\mathbf{j} = -\sigma \nabla \phi \quad \text{(4)}
\]

Where \( \phi \) is the electric potential. Substituting Equation (4) into Equation (3) and discretizing it using an MPS (Moving Particle Semi-implicit) method [22], the following equations can be written.

\[
\frac{2d}{\Sigma_b |\mathbf{r}_{ab}|^2} W_{ab} \sum_b m_b \frac{2 \sigma_a \sigma_b}{\rho_a \rho_b} (\phi_b - \phi_a) W_{ab} = 0
\]

\[\text{(5)}\]

\[
\phi_a^{n+1} = \frac{\Sigma_b \sigma_b \phi_b W_{ab}}{\Sigma_b \sigma_b W_{ab}}
\]

\[\text{(6)}\]

\( n \) is the number of iterations. The potential of the particles is repeatedly updated using Equation (6) until the sum of all particles in the residual of Equation (5) is less than or equal to 1% of the current flowing through the entire materials to be welded. Then, using the potential obtained from this convergence calculation and Equation (4), the current density at the location of each particle can be determined. The magnetic flux density can be obtained from Equations (7) and (8).

\[
\mathbf{B} = \nabla \times \mathbf{A} \quad \text{(7)}
\]

\[
\nabla \times \mathbf{A} = -\mu_0 \mathbf{j} \quad \text{(8)}
\]

Where \( A \) is the vector potential and \( \mu_0 \) is the magnetic permeability of the vacuum. By applying the discretization technique of the MPS method, Equation (8) is discretized as follows.

\[
\frac{2d}{\Sigma_b |\mathbf{r}_{ab}|^2} W_{ab} \sum_b \left( \mathbf{A}_b - \mathbf{A}_a \right) W_{ab} = -\mu_0 \mathbf{j} \left( \mathbf{r} - \mathbf{r}_a \right)
\]

\[\text{(9)}\]

\[
\mathbf{A}_a = \frac{\sum_b \mathbf{A}_b W_{ab} + \sum_a \frac{|\mathbf{r}_{ab}|^2}{2d} W_{ab} \mathbf{j} \left( \mathbf{r} - \mathbf{r}_a \right)}{\sum_b W_{ab}}
\]

\[\text{(10)}\]

Using Equation (10), a variant of Equation (9), the vector potential of particle \( a \) at position \( \mathbf{r} = \mathbf{r}_a \) is iteratively updated.

In this study, it is assumed that Fe2Al5 formed in the temperature range higher than the melting point of aluminum alloys (880 K) grows as an intermetallic compound layer and its formation in the thickness direction follows the parabolic law shown in Equations (11) and (12) [2].

\[
Z_{r_i} = \sqrt{2k_{r_i} t_s}
\]

\[\text{(11)}\]

\[
k_{r_i} = k_0 \exp \left( -\frac{Q}{RT_{r_i}} \right)
\]

\[\text{(12)}\]

\( Z_{r_i} \) is the thickness of the intermetallic compound layer at position \( \mathbf{r} = \mathbf{r}_i \) at the junction interface, \( k \) is the reaction rate constant, \( t_s \) is the reaction time, \( k_0 \) is the frequency factor, \( Q \) is the activation energy, \( R \) is the gas constant, and \( T_{r_i} \) is the temperature at the position \( \mathbf{r}_i \) at the junction interface. The frequency factor \( k_0 \) is \( 3.79 \times 10^{-6} \text{ m}^2/\text{s} \), the activation energy \( Q \) gives 120 kJ/mol [2]. The increase in the thickness of the intermetallic compound is determined by Equation (13), which is obtained by differentiating Equation (11) by substituting Equation (12). \( dZ_{r_i} \) is the increase in the thickness of the intermetallic layer at position \( \mathbf{r}_i \) over a small time \( dt \). Integrating \( dZ_{r_i} \)
from the start of the computation to an arbitrary time gives the thickness of the intermetallic compound layer at that time.

\[
dZ_{ri} = \frac{k_b}{2\tau_i} \exp\left(-\frac{Q}{RT_{ri}}\right) dt \quad (13)
\]

### 2.2. Computational domain and computational conditions

Figure 1 shows the computational domain, with the black area representing the electrode, the dark gray area representing mild steel, and the light gray area representing an aluminum alloy. The computational domain is three-dimensional, and the Cartesian coordinate system is set. The contact surface between the mild steel and aluminum alloy is located at \( z = 1.9 \text{ mm} \). The electrode and materials to be welded consist of 119,496 particles with a diameter of 0.1 mm. Table 1 shows material properties used in this study. Density, specific heat, and thermal conductivity are assumed to be those of mild steel and 5000-series aluminum alloys, and values at 300 K are given for both materials [23,24].

Melting of mild steel, the latent heat of fusion for mild steel is 250 kJ/kg and that for aluminum alloys is given as 400 kJ/kg. A phase change is assumed to occur when a particle that has reached the melting point receives half the energy of the latent heat of fusion [25]. The electrical conductivity of mild steel is \( 1.0 \times 10^6 \text{ S/m} \), and that of aluminum alloy is assumed to be \( 2.0 \times 10^6 \text{ S/m} \). For simplicity, it is assumed that the electrode temperature is fixed at 300 K, assuming that it is water-cooled, and the surface where the electrode contacts the material to be welded is flat. In reality, a temperature rise of the electrode is considered to exist, but since this computation does not consider the temperature dependence of physical properties, the effect on the current path, etc., is assumed to be small. The potential of each electrode is the potential of the material to be welded when viewed along the \( z \)-axis. The potential of the top electrode is fixed at 1.5 V and that of the bottom electrode is fixed at 0 V. In this study, computations are performed for 100 ms with a time step of 0.05 ms, and energization is performed at the start of the computation. The computation time consists of 40 ms for the energization time and 60 ms for the de-energization time, which assumes the pressurization holding time and cooling time in the execution.

The assumptions for the computations in this study are shown below. For simplicity, the pressure of materials to be welded by the electrode is not considered in this study, and the solid region is assumed to be undeformed. The Joule heat generated by the current flowing between the electrodes is considered for the entire the materials. The contact electrical resistance is calculated using the model developed by Babu et al. [26], and it is assumed that heat is generated only in the region of contact between solid materials to be welded. The heat generated on the contact surface between the material to be welded and the electrode shall not be considered.

### 3. Computational results and discussion

#### 3.1. Nugget formation process during resistance spot welding of dissimilar materials

Figure 2 shows the nugget formation process from the start of energizing and the cooling process of the nugget after the end of energizing, showing (i) the particle state distribution and (ii) the temperature distribution at each time in the \( xz \) section through the electrode center axis. The color of each particle in the particle state distribution represents the electrode in black, solid mild steel in dark gray, solid aluminum alloy in light gray, molten mild steel in red, and molten aluminum alloy in
blue. On the other hand, in the temperature distribution, particles are colored from blue to red according to their temperature.

After the start of energizing, the temperature rises at the joint interface due to Joule heating and heat generated by contact resistance, and the aluminum alloy melts first. On the other hand, melting of mild steel begins near the center of the plate in the thickness direction (Figure 2(a)). Thereafter, as time passes, the molten area of the aluminum alloy increases at the joint interface, and the nugget grows in the direction of the plate thickness. In contrast, the nugget of mild steel expands in an ellipsoidal shape from the center of the plate in the thickness direction (Figure 2(b)). This is because the thermal energy generated at the joint interface on the mild steel side is transported to the aluminum alloy side by thermal conduction. In addition, the temperature distribution in the middle of the mild steel plate in the thickness direction shows a high temperature exceeding 1,700 K due to Joule heating. During the non-energizing period after 40.0 ms from the start of energizing, no heat is generated by Joule heating or contact resistance, and solidification begins as a result of cooling. Solidification of the mild steel nugget begins at the solid-liquid interface, and since the electrode is water-cooled and the temperature is fixed at 300 K, the solidification of the upper nugget near the electrode is earlier than that of the lower nugget in the mild steel nugget. Similarly, solidification of aluminum alloy nugget progresses from the bottom of the nugget near the electrode.

Figure 3 shows the velocity distribution of particles constituting the nugget during the energization period. The figure is an xz cross section through the electrode center axis. The color indicates the magnitude of the velocity, and the direction of the arrow indicates the direction of the velocity vector. To obtain this figure, a grid with the same spacing as the particle diameter is created on the computational domain where the particles are located, and the kernel averaging process [14] is performed at every grid point. Thereafter, this velocity field is then obtained by time averaging using the results of the kernel averaging process for 5-time increments. Therefore, this velocity distribution of the molten metal is spatially and temporally averaged.

The white line in the figure indicates the boundary of the nugget region. In the case of mild steel nugget, no flow velocity distribution is observed, but in the case of aluminum alloy nugget, the molten metal flows from the periphery to the center at the bottom of the nugget, flows from the bottom to the top at the center of the nugget, and then forms a velocity distribution near the joint interface that flows from the center to the periphery (Figure 3(b)). This is due to the electromagnetic force acting
within materials to be welded. Figure 4 shows the distribution of the electromagnetic force acting on the particles constituting the nugget during the energization period. Figure 4(a) and Figure 4(b) correspond to Figure 3(a) and Figure 3(b), respectively. As in Figure 3, this figure also shows the xz section through the electrode center axis. The color indicates the magnitude of the electromagnetic force, and the direction of the arrow indicates the direction in which the electromagnetic force acts. The figure shows that the electromagnetic force acts toward the center of the nugget. The electromagnetic force is small around the center of the nugget and is large near the edge of the nugget. This is attributed to the small magnetic flux density in the central zone of the nugget and the large one near the edge of the nugget. In Figure 4(b), where the nugget has grown significantly, the electromagnetic force near the edge of the nugget is slightly larger on average than that at the joint interface as the nugget grows closer to the electrode. In consequence, an upward velocity from the bottom to the top of the nugget was generated inside the nugget on the aluminum alloy side. On the other hand, because the nugget diameter is smaller and the density of the mild steel is larger inside the nugget on the mild steel side, the acceleration inside the nugget on the mild steel side is smaller than that inside the nugget on the aluminum alloy side, even if the same volumetric force is applied, and the driving force is not enough to produce a flow.

Figure 5 shows the heat distribution by heat conduction during the energization period. Figure 5(a) and 5(b) correspond to Figure 3(a) and 3(b), respectively, showing the xz cross section through the electrode center axis as in Figure 3. The color of a particle indicates the magnitude of its heat conduction. Both figures show that heat transport by heat conduction is greater in the molten aluminum alloy. This is because the relatively low-temperature molten metal below the nugget is transported to the top of the nugget by molten metal convection caused by electromagnetic forces, as described in Figures 3 and 4, and heat transport occurs...
between the relatively low-temperature molten metal below the nugget and the surrounding high-temperature molten metal.

3.2. Temperature history and growth of intermetallic compound layer at joint interface during dissimilar material resistance spot welding

Figure 6 shows the nugget shape of the aluminum alloy at the end of energization ($t = 40.0 \text{ ms}$). Point A to E shown in this figure ($x = 1.0, 2.0, 3.0, 4.0, 5.0 \text{ mm}$, $y = 3.0 \text{ mm}$, $z = 1.9 \text{ mm}$) are temperature acquisition positions. Figure 7 shows the temperature history of the contact interface between the mild steel and the molten aluminum alloy at points A to E. During the energized period from the start of this computation to $t = 40 \text{ ms}$, the temperature at each point increases due to Joule heating and heat generated by contact resistance, followed by a decrease in temperature during the no-energized period to 100 ms. Figure 8 is obtained using the temperature histories of the points A to E obtained from Equation (13), and shows (a) the thickness of the intermetallic compound with time evolution and (b) the thickness distribution of the intermetallic compound at $t = 100 \text{ ms}$. Figure 8(a) indicates that the intermetallic compound thickens in the interval from $t = 20 \text{ ms}$ to 60 ms, when the temperatures at each measurement point sequentially exceed the melting point of the aluminum alloy. Figure 8(b) suggests that the intermetallic compound tends to be thicker near the center of the aluminum alloy interface and thinner at the interface edge. Furthermore, the thickness is about 1 $\mu$m [2,3] as with the experiment, which is a reasonable value.

Thus, the nugget formation process in resistance spot welding of dissimilar materials is successfully simulated using the computational model of the melting and solidification process that takes convective heat transport into account.
account developed in this study by the incompressible SPH method. It is also shown that it is possible to estimate the thickness of the intermetallic compound layer reasonably from the obtained temperature history.

4. Conclusions

In this study, the melting and solidification processes of mild steel and aluminum alloys were modeled and numerically simulated by considering convective heat transport using the incompressible SPH method for resistance spot welding of dissimilar materials. Furthermore, the temperature history of the joint interface was obtained from the simulation results, and the thickness of the intermetallic compound layer was estimated. The following are the main findings.

1. The aluminum alloy began to melt from the joint interface, and the melting area expanded in the direction of the plate thickness. On the other hand, the mild steel melted from near the center of the plate in the thickness direction, and the molten area became an oval sphere.

2. During the energization period, heat transport by heat conduction increased in the molten aluminum alloy. This was thought to be due to the convection of the molten metal caused by electromagnetic forces, which transported the relatively cold molten metal below the nugget to the top of the nugget and enhances heat transport to and from the surrounding high-temperature molten metal.

3. The thickness of the intermetallic compound layer was estimated from the temperature distribution obtained by the computations. The thickness of the intermetallic compound layer tended to be thicker at the center of the joint interface and thinner at the edges.

4. The thickness of the intermetallic compound layer obtained by this computation was about 1 μm, which was a reasonable value as obtained experimentally. Therefore, it was possible to estimate the nugget formation process and the thickness of the intermetallic compound layer in dissimilar material resistance spot welding using the computational model developed in this study.

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