Molten-Shape Prediction and Fracture-Life Evaluation of Micro-Solder Joint in Semiconductor Structure*

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Abstract
The reliability of a micro-solder joint in a semiconductor structure depends on its solder shape. Therefore, many methods of predicting the molten-solder shape have been proposed. However, conventional methods cannot be used to accurately predict the shape of a miniaturized solder. In a miniaturized solder joint, molten solder greatly changes its shape during the reflow process, and even topology changes (e.g., merging with another solder in a neighboring joint or splitting into several pieces) might occur. Conventional methods cannot be used for expressing these phenomena. To predict a miniaturized solder shape, we developed a new shape-prediction method based on the moving-particle semi-implicit (MPS) method. In the MPS method, a continuum is expressed as an assembly of particles. In contrast to finite element analysis (FEA), our new method can easily express large deformation and topology changes because the continuum does not need to be divided into elements. Moreover, we evaluated the fracture life of a solder joint with the predicted solder shape by coupling our shape-prediction method with a crack-propagation analysis method that we also developed. The crack-propagation is used for automatically calculating a crack-initiation point and crack-propagation paths, and the fracture life is evaluated quantitatively. We applied this coupling method to evaluate fracture lives of various solder joints and found that a difference in solder shape caused a difference in crack-initiation points, crack-propagation paths, and fracture lives.

Key words: Shape Prediction, Molten Solder, MPS Method, Life Prediction, Crack Propagation, Finite Element Method

1. Introduction

In semiconductor products, various solder-joint structures have been used for connecting a board to a semiconductor package. Fig. 1 shows two examples of solder-joint structures. Fig. 1(a) shows a solder joint in a thin-small-outline-package (TSOP) structure, and Fig. 1(b) shows a solder joint in a ball-grid-array (BGA) structure. In Fig. 1(a), a solder climbed up a lead terminal of a package and connected the lead terminal to the board. In Fig. 1(b), a solder ball with a void connected the substrate to the board.

Fig. 2 indicates the functions of a solder. In a semiconductor package, a chip is arranged on a substrate with a die attach film (DAF) and connected by wire to the substrate electrically. In this case, there are mainly three functions of a solder joint. The first function is an electrical connection. To enable the operation of a chip, a solder joint should
connect a semiconductor package and a board electrically. The second function is a thermal connection. Because the temperature of a chip rises while a semiconductor is operating, a solder joint should conduct heat from a semiconductor package to a board for dissipating heat. The third function is a mechanical connection. To fix a semiconductor package onto a board, the solder joint should connect them mechanically.

When a solder joint fractures, a micro-crack is generated in the start as shown in Fig. 3(a), a crack propagates afterwards, and it finally becomes a fracture as shown in Fig. 3(b). Because the three functions mentioned above are not lost only by a micro-crack generation, a solder-joint lifetime is defined not by micro-crack generation but by joint fracturing. As a result, we have to investigate crack propagation characteristics to estimate solder-joint lifetime.

Fig. 4 and 5 show the trends of solder joints. Fig. 4 shows the trend of the pitch of the solder ball terminal in plastic-molding packages by using package-dicing technology (1). The figure shows that the miniaturization of solder joints advances every year. Fig. 5 shows the trend of lead free solder joints. The shift to lead-free material in low-melting solder has already been completed due to the “restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)” (2). Although high-melting solder has been excluded from RoHS, it is thought that lead-free high-melting solder will also be required in several years.
In miniaturized joints, the shape of molten solder changes greatly during the reflow process. Furthermore, topology changes can occur because the space between solder joints is small. Also, the wettability of lead-free solders is different from conventional solders. These phenomena make solder-shape prediction difficult.

We developed a new shape-prediction method for miniaturized and lead-free solder. Furthermore, we demonstrated a fracture-life evaluation of solder joints by coupling our shape-prediction method and a crack-propagation analysis method that we also developed.

2. Shape-prediction method

Many methods for predicting molten solder shapes have been proposed. Kitano et al. (3) proposed a method to obtain a theoretical solder shape to satisfy the mass conservation condition and equilibrium of force (surface tension, gravity, and external force). This is a powerful method to predict a simple solder shape like an axisymmetric solder bump in a BGA package. However, it is difficult to predict complex shapes. Nagata et al. (4) proposed a method using finite element analysis (FEA) by assuming molten solder to be a viscous fluid. The method proposed by Brakke et al. (5) also uses FEA to predict not only the solder shape but also the rigid deformation of the semiconductor package. FEA is effective in expressing complex solder shapes easily because a solder joint is divided into many primitive elements and the solder deformation is expressed as the sum of the element deformations. However, it is difficult to express topology changes and large deformations. Therefore, it is necessary to develop a new solder shape prediction method that can express these factors.

To express topology changes and large deformations, we proposed a new solder shape prediction method by using the particle method. In the particle method, a continuum is expressed as an assembly of particles that represent neighborhood properties, and a
continuum motion is expressed by the sum of the particle motions. Because a continuum is divided into elements, FEA cannot express large deformation e.g. deformation that the angle in an element becomes 0 degrees or less or 180 degrees or more. Because a continuum need not be divided into elements in the MPS method, topology changes and large deformations can be expressed easily.

Many particle methods have been proposed, so we used the moving-particle semi-implicit (MPS) method proposed by Koshizuka et al. \(^{(6,7)}\). The MPS method is suitable for calculating incompressible flow, so we speculated that it would also be suitable for expressing molten solder characteristics in the reflow process. The characteristics of molten solder greatly depend on its wettability. This feature is different from other conventional incompressible flows. However, the original MPS method cannot sufficiently express the effects of wettability. Therefore, we enhanced the surface tension formulation of MPS, enabling us to express these effects.

In this paper, the explanation of the calculation technique of general incompressible flow characteristics \(^{(4)}\) was omitted. We focused instead on explaining the surface tension calculation technique that was enhanced to express the effects of wettability. Surface tension \(f\) is expressed by the following equation.

\[
f = \frac{1}{\rho} \sigma \kappa \delta \mathbf{n}.
\]

Here, \(\rho\), \(\sigma\), \(\kappa\), \(\delta\), and \(\mathbf{n}\) are density, surface tension coefficient, curvature factor, delta function for defining a surface, and directional vector, respectively. Density \(\rho\) and surface tension coefficient \(\sigma\) were defined by material and environmental conditions. Curvature factor \(\kappa\) was calculated by counting particles that were near the focal particle. Fig. 6 depicts the surface near focal particle \(i\). Particles whose distance from point \(i\) was \(r_e\) or less were counted, and it was determined that the larger the number of counted particles, the larger the angle \(\theta\) was. Therefore, \(\kappa\) is expressed by the following equation,

\[
\kappa = \frac{2 \cos \theta}{r_e}. \tag{2}
\]

The directional vector \(\mathbf{n}\) was calculated by counting the particles that were near the adjacent points of particle \(i\). The particle density gradient at the position of particle \(i\) can be calculated by using the number of counted particles. Therefore, \(\mathbf{n}\) was calculated using the gradient information.

It is important to note that \(\kappa\) and \(\mathbf{n}\) are different in wettability conditions. However, they cannot be expressed using the above technique. Therefore, we defined the weight that shows the wettability of each material. When calculating \(\kappa\) and \(\mathbf{n}\), the weight of each particle is counted instead of the particle itself. Fig. 7 illustrates the solder shapes with the highest and lowest wettability. Fig. 7(a) shows the solder shape in which the weight of all particles are the same (all weight 1.0), and Fig. 7(b) shows the solder shape when the weight of the solder particles is 1.0 and the weight of the land particles is 0.0. In Fig. 7(a), neither solder particles nor land particles were distinguished when calculating \(\kappa\) and \(\mathbf{n}\). As a result, the solder surface was shaped by both the land particles. This is the highest wettability condition. In Fig. 7(b), the land particles were ignored when calculating \(\kappa\) and \(\mathbf{n}\). As a result, the solder surface was shaped by only the solder particles. This is the lowest wettability condition. As above, the solder shape with each wettability condition can be obtained by defining the particle weight. In addition, this technique can also be used to express a slight difference in the wettability, although Fig. 7 shows two extreme conditions.
3. Verification of prediction

The validity of solder shape prediction was verified by using the example shown in Fig. 8. The object of analysis was a circular ball of solder on a flat land. In this example, a molten steady shape was predicted and compared with the theoretical shape. In this calculation, the effect of temperature change is not considered and the values of density, surface tension and wettability are fixed. This is a calculation to which a steady shape in the reflow temperature condition is obtained.

This shape was defined as the shape when the solder deformation velocity is below the specified value. The weight of the solder and land particles was defined as 1.0, and that of the solder resist particles was 0.0. Density was $8.5 \times 10^{-6} \text{ kg/mm}^3$, surface tension was $3.2 \times 10^{-4} \text{ N/mm}$, and the initial distance between each particle was 25 $\mu\text{m}$. The analysis was implemented by using our own coding program.

Fig. 9 illustrates the predicted shapes when the initial solder diameters are 0.3, 0.5, and 0.7 mm. In each case, the solder covered the high-wettability land and did not touch the low-wettability solder resist. These results show that our developed method can express the difference in wettability. Fig. 10 shows the theoretical shapes calculated by Kitano’s method (1) and Fig. 11 shows the relationship between the height of the steady shape and initial solder diameter. The shapes predicted using the developed method corresponded to the theoretical shapes. These results indicate that the predictions using our developed method are reasonable.

In this paper, predicted shapes were compared with the theoretical shapes. The comparison with other predicted methods are future tasks.

4. Example of shape prediction

4.1 Example 1: Solder joint in TSOP package

The developed method was applied for calculating the solder shapes of the TSOP package shown in Fig. 12. In this example, only the solder particles were removable, and the other particles (lead, resin and solder resist) were fixed. The wettability of the land was
high, that of the solder resist was low, and that of the lead was variable (the lead weight was 0.0-1.0). The initial distance between each particle was 10 μm.

Fig. 13 shows the analysis results when the lead had high wettability. The solder climbed up the lead in a steady state, even though the initial solder shape was flat against the land. Fig. 14 shows the steady solder shapes in various wettability conditions. With higher wettability of the lead, the solder shape climbed up more. If the wettability of the lead was lower, the contact angle between the solder and the lead was larger. Thus, our developed method can be used for expressing complex solder shapes in various wettability conditions.
4.2 Example 2: Solder joint in flip-chip package

Next, the developed method was applied for calculating the solder shapes of stud bumps in a flip-chip package as shown in Fig. 15. In this example, two lands were covered with solder in the initial shape. The wettability of the stud bumps and the land was high and that of the solder resist was low.

Fig. 16 depicts the analysis results. Although the initial solder was in one “piece,” it split in two and climbed up each stud bump. Thus, our developed method can be used for easily expressing topology changes like splitting.
4.3 Example 3: Self-Alignment effect of solder ball in BGA package

In examples 1 and 2, only the shape of the solder was changed and the other materials were fixed. However, it is also possible to move other materials by using the MPS method. Therefore, we demonstrated the self-alignment effect of a solder ball; that is the effect of automatically correcting the position by the surface tension of solder. The position of a semiconductor package was offset before the reflow process as shown in Fig. 17(a). The package was moved by the surface tension of the solder, and the position was corrected after the reflow process as shown in Fig. 17(b).

Fig. 18 shows the result of the demonstration. Although the positions of the upper and lower lands were offset for the initial shape, the positions aligned after calculation. Thus, our developed method can be used for expressing the self-alignment effect and the package movement.
5. Evaluation of fracture life

Evaluating the fracture life of a solder joint including the effect of wettability is possible by combining our shape-prediction method with our crack-propagation analysis method. Fig. 19 is a flowchart of our crack-propagation analysis (8). In our method, crack-initiation point and crack-propagation behavior are evaluated quantitatively based on the damage that accumulates during fatigue test. The accumulated damage is estimated by using the Coffin-Manson’s law and the Miner’s rule. Fig. 20 shows the comparison between analysis result and measured crack behavior (8). Analysis object is a solder ball joint under a forced shearing displacement. Detailed analysis conditions are described in (8). Fig. 20(a) shows the calculated crack-propagation path. The crack propagates near the interface between solder and land, but does not propagate to the interface itself. This feature is corresponding to the measured crack path shown in Fig. 20(b). Fig. 20(c) shows the estimated fracture life and measured fracture life. We can find that the fracture life can be estimated quantitatively.

Fig. 21 is an example of the analysis results of a thermal fatigue test. Temperature change in 25, -25, 125, and 25 degrees is defined to be one cycle. The analyzed object was a TSOP package whose left consisted of high wettability lead and whose right side consisted of low wettability lead. First, shape prediction analysis was done. Next, the models were converted into an FE model. Finally, crack-propagation analysis was
Figure 19: Flowchart of crack propagation analysis

performed. The conversion method of analysis model is as follows. First, lattice cell is piled up to the calculated solder shape. Next, the cell to which it is occupied more than the half with solder is sorted out. Next, sorted cells are converted into finite elements.

After 1000 cycles, a micro-crack was generated at the solder fillet on the left side (high wettability side). This crack-initiation point is near the center of the solder fillet and this point is corresponded to the actual point (9). On the right side (low wettability), a crack was generated and propagated at the interface of the solder and the lead. After 3300 cycles, a crack was propagating at the interface on the left side, although it had not yet fractured; on the right joint, however, a fracture occurred.

In the low wettability conditions, as the contact angle between the solder and the lead increases, the strain singularity at the interface increases. As a result, the crack was generated at an early cycle. Furthermore, the difference in the crack initiation cycle caused a difference in joint stiffness on each side, and the crack propagation on the side with low stiffness (right side) was accelerated. These phenomena caused the difference in the fracture life of the solder joint.

6. Conclusion

(1) We developed a new shape prediction method for molten solder joints using the MPS method. Our developed method can be used for easily expressing topology changes, large deformations, and the effects of wettability.

(2) We found not only the solder shapes of TSOP and FC but also the self-alignment effect of solder ball and the package could be predicted by using our developed method.

(3) We evaluated the fracture life of a solder joint with the predicted solder shape by combining our shape-prediction method with our crack-propagation analysis method. We found the differences in crack initiation points, the crack-propagation paths and fracture lives in different wettability conditions.
Using the combination of the shape-prediction method and the crack propagation analysis, we enabled to analyze the phenomena from manufacturing process to product lifetime.

References

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Figure 20: Comparison between analysis result and measured crack behaviour
Figure 21: Flow of fracture-life evaluation