

Numerical simulation of the atomic migration and diffusion during current stressing in the Cu/Sn-58Bi/Cu solder joints

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Abstract

In this work, we tried to use the finite element analysis (FEA) method to simulate the atom migration during current stressing at different temperatures. Based on the FEA tool of ABAQUS, the heat transfer subroutine of UMATHT was secondary developed, establishing the corresponding relationship between heat transfer and classical diffusion theory. The Bi migration content with current stressing time was given. Results showed that the Bi content at the anode interface increased upon the stressing time. Moreover, the Bi migration rate underwent a sharp increase at the initial stage as the EM effect occurred, and then dropped and tended to be stable. When the stressing time was up to 48h, the Bi content at the anode interface could reach 97%, which definitely proved that most Bi atoms had migrated and aggregated at the anode interface to form a continuous Bi layer. Furthermore, the experimental test was conducted with the same EM condition. EDX analysis results indicated that the Bi content at the anode after current stressing for 48h was in accordance with the simulation results, which validated the simulation method.

Introduction

The electromigration (EM) behavior of the Cu/Sn-58Bi/Cu solder joint has been widely investigated, mainly focusing on the experimental method. Results indicate that many influencing factors may affect the EM reliability of the solder joints, including current density, loading temperature, temperature gradient, chemical gradient and so on [1-3]. It has been pointed out that the atoms will migrate and diffuse along the electron direction, leading to the void or crack formation at the cathode interface and hillock or whisker formation at the anode interface [4, 5]. Similar work has been done in our group with various experimental conditions, focusing on the atom migration mechanism at different current densities and loading temperatures [6-8]. However, due to the different geometry of the tested samples and experimental conditions and the potential defects in solder matrix, the real EM behavior will be affected by these complicated factors, maybe resulting in the deviated conclusion. Therefore, finite element analysis method was used by many investigators to analyze the EM behavior from the aspect of the current density distribution, thermal stress distribution, temperature distribution, void propagation and so on.

In this paper, the atom migration behavior was simulated by the finite element analysis method during current stressing process at different temperatures in Cu/Sn-58Bi/Cu solder joint. Based on the FEA tool of ABAQUS, the heat transfer subroutine of UMATHT was secondary developed, establishing the corresponding relationship between heat

transfer and classical diffusion theory. The Bi and Sn migration content with current stressing time was given. Furthermore, to verify the simulated results, the EM test with the same experimental condition was conducted. The one-dimensional solder joint of Cu/Sn-58Bi/Cu was stressed at the current density of 10^4A/cm^2 at room temperature and high temperature (55°C).

Experimental

First of all, based on the FEA tool of ABAQUS, the heat transfer subroutine of UMATHT was secondary developed, establishing the corresponding relationship between heat transfer and classical diffusion theory (based on the Fick law: concentration gradient typed diffusion), which the main analogy relationship between them is shown in Tab.1 [31]. The Bi and Sn migration content with current stressing time was calculated.

Tab.1 Relationship between heat transfer analysis and heat diffusion analysis

Heat transfer analysis		Heat diffusion analysis	
Variable	Description	Variable	Description
U(θ)	Internal energy	U(c)	Chemical potential
T	Temperature	C_L	Gradient
Cp	Specific heat	D_L/D_{eff}	Effective diffusion constant
ρ	Density	1	Uniformity
k	Conductivity	D_L	Diffusion rate

Secondly, the EM test was conducted with one-dimensional Cu/Sn-58Bi/Cu solder joints. After EM test, an energy dispersive X-ray spectroscopy (EDX) system was used to detect the element distribution. Detail EM sample fabrication procedures are as follows. The oxygen-free high-conductivity copper sheet with a thickness of 0.5 mm was cut into 25×2 mm strips by electro-spark discharge machining (EDM). Before soldering the joints, these Cu substrate specimens were cleaned by dipping them into 30 % nitric acid solution for 1 min followed by acetone rinse and drying. The Sn-58Bi solder alloy was fabricated by alloying method. During the alloying process, ceramic crucible was used as container. After the melting of the solder, the liquid was casted into a rod ingot, followed by being rolled into sheets with different thickness according to the experimental requirement.

Thickness of solder sheet can be further precisely controlled by the spiral micrometer. One solder disk and two Cu stripes were placed into an aluminum elbow-bracket. With the help of

a stereo microscope, the solder disk was stuck between two Cu stripes, which were then fastened against the walls of the elbow bracket by bolts. Furthermore, a K-type thermocouple was fixed near the soldering region. It should be pointed out that the intersection angle between two coppers is 90°, meanwhile, the two ends of the solder joint was bended to 90° after soldering, then place it in the epoxy resin to inlay. After polishing the inlaid solder joint, the final morphology of the solder matrix can be obtained. Grinding machine was applied to reduce the dimension of the samples, followed by grid sandpapers, and finely polished with Al₂O₃ suspension.

Results and discussion

In ABAQUS software, UMATHT as the user subroutine is widely used for constructing the constitutive equations in thermodynamics of material, which can define the character of the material thermodynamic and the internal thermal property during thermal conduction. It should pre-define the internal energy per unit mass of the material, the thermal flux vector, and the differential for the temperature and the temperature gradient. Furthermore, update the variable related with final solve of the subroutine after each increment [1].

Heat transfer control equation in UMATHT is expressed as the following:

$$U(\theta) = U_0 + dU - Qdt / \rho - vdt \times (C_p + \theta dk / d\theta) \times (d\theta / dx) \quad 1-1$$

In this formula, U is the total system energy, U_0 is the initial system energy, Q is the internal heat source, ρ is the material density, θ is the temperature, $C_p = du/d\theta$ is the specific heat, v is the moving speed of the internal heat source. The formula includes four parts, the first part is the initial energy, and the second one is the energy increment, the third part is energy change induced by the internal heat source, the forth part is the energy change induced by the movement of the internal heat source. Therefore, if the system doesn't have the internal heat source, the third part and the forth part should be omitted. Then the formula 1-1 can be simplified as formula 1-2:

$$U(\theta) = U_0 + dU \quad 1-2$$

We establish the relationship between heat transfer and diffusion based on the variable substitution in Tab.1 The classical diffusion control equation can be expressed in UMATHT:

$$U(c) = U_0 + dU \quad 1-3$$

In this formula, $U(c)$ is the total system chemical potential, U_0 is the initial chemical potential, c is the concentration.

The back stress is comparatively low than the electron wind force during Bi atoms diffusion process. So this back stress can be ignored, the diffusion flux equation can be expressed as formula 1-4.

$$J_{em} = V_{em} / \Omega \cdot (A \cdot t) \approx C \cdot \frac{D}{kT} \cdot Z^* \cdot e \cdot E \quad 1-4$$

Chin-Ming Chen [9] pointed out that the atom diffusion phenomena accompanied with large Joule heating, the product of the Bi atom diffusivity and the effective charge number ($D \cdot Z^*$) gradually increased. We found out that the $D \cdot Z^*$ increased from $1.74 \times 10^{-10} \text{ cm}^2/\text{s}$ to $6.28 \times 10^{-10} \text{ cm}^2/\text{s}$ as the current density increased from $5 \times 10^3 \text{ A/cm}^2$ to $6.5 \times 10^3 \text{ A/cm}^2$.

Because of higher resistivity of the Bi layer than the eutectic SnBi, leading to more Joule heating accumulation at the anode interface to further promote the Bi layer growth. In this paper, the product of the $D \cdot Z^*$ can be obtained by interpolation method which the data rooted in reference [9] as shown in Fig.1.

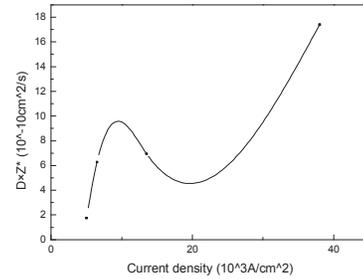


Fig.1 Relationship between the current density and the $D \cdot Z^*$

In our one-dimensional solder joint, the electric potential (E) varies linearly along the current direction, which can be shown in formula 1-5.

$$E = \frac{x}{l} \cdot E_0 \quad 1-5$$

Which x is the distance along the current direction, l is the length of the solder matrix between two Cu substrates, E_0 is the total electric potential difference between cathode and anode.

$$E_0 = I \cdot R = I \cdot \Omega_{Bi} \cdot \frac{l}{A} = \left(\frac{l}{A}\right) \cdot \Omega_{Bi} \cdot l = J \cdot \Omega_{Bi} \cdot l \quad 1-6$$

Which A is the cross-sectional area of the solder joint, Ω_{Bi} is the resistivity of the Bi, J is the current density. Combine formula 1-6 and 1-5, we can get the final electric potential expression as shown in formula 1-7.

$$E = J \cdot \Omega_{Bi} \cdot x \quad 1-7$$

Different from the classical diffusion theory which the concentration gradient provides the driving force, the electron wind force takes the main driving force during the electromigration process. We take the electric potential as the influencing factor to the diffusion coefficient of D' :

$$D' = \frac{D}{kT} \cdot E \quad 1-8$$

$\frac{D}{kT}$ is the atom migration ability. Combine with formula 1-4, the J_{em} can be expressed as formula 1-9.

$$J_{em} = Z^* \cdot e \cdot D' \cdot C \quad 1-9$$

We ignore the influence of the IMC evolution and phase transition, only establish the model of the Sn-58Bi solder matrix. The structured mesh generation is used, and set the global element as $2 \times 10^{-5} \mu\text{m}$. DCC3D8 typed liner heat transfer/diffusion element is adopted. Load electric potential of 0 and E_0 on both sides of the solder matrix. Combine formula 1-3 with 1-9 to compile the subroutine and simulate the Bi element diffusion process. Fig.2 shows the Bi content evolution with current density of 10^4 A/cm^2 with stressing time up to 48h at the anode. Simulated results show that the Bi content at the anode interface increases as the stressing time goes up. Moreover, the Bi migration rate undergoes a sharp increase at the initial stage as the EM effect occurs, and then drops down and tends to be stable. When the stressing time is

up to 48h, the Bi content at the anode interface is about 97%, which definitely proves that most Bi atoms have migrated and aggregated at the anode interface to form a continuous Bi layer.

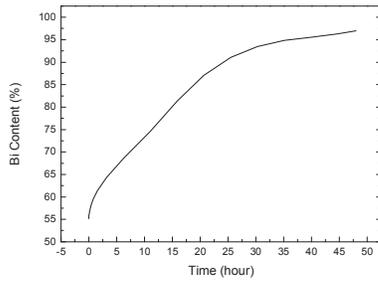


Fig.2 The profile of the Bi content evolution with stressing time at the anode

Fig.3 shows the simulated result of the Bi element distribution along the current direction with the same current density under 20°C and 55°C, respectively. We can see that Bi migration rate can accelerate as the temperature increases. We all know that the electromigration induced mass flux has great relation with the temperature. As the temperature goes up, the coefficient of effective diffusion will increase, leading to accelerate the atom migration rate. This is in accordance with the simulated result.

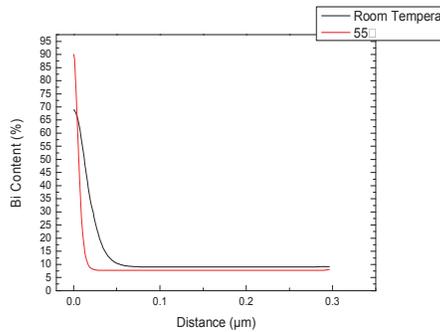


Fig. 3 Bi element distribution along the current direction under 20°C and 55°C

Fig. 4 shows Bi element distribution along the current direction by EDX and simulated methods. These two results are well matched that the Bi content presents gradient distribution along the current direction in the solder matrix, and form a thick Bi layer at the anode.

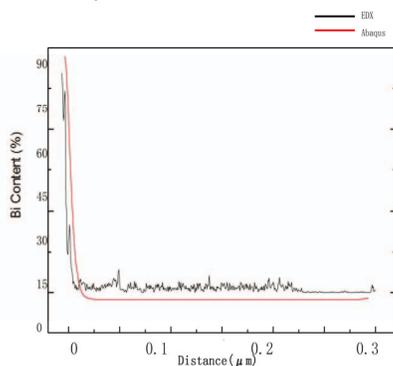


Fig. 4 Bi element distribution along the current direction by EDX and simulated methods

Conclusions

The Bi migration content with current stressing time was simulated by ABAQUS software. Results indicated that the Bi content at the anode interface increased as the stressing time increased. Initially, the Bi migration rate underwent a sharp increase then dropped down and tended to be stable. As the stressing time was up to 48h, the Bi content at the anode interface could reach 97%, which definitely proved that most Bi atoms had migrated and aggregated at the anode interface to form a continuous Bi layer. EDX analysis results indicated that the Bi content at the anode after current stressing for 48h was in accordance with the simulated results, which validated the simulation method.

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References

1. C. M. Chen and C. C. Huang, "Atomic migration in eutectic SnBi solder alloys due to current stressing", *J. Mater. Res.*, Vol. 23, No. 4 (2008), pp. 1051-1056
2. X. Gu, Y.C. Chan, "Electromigration in Line-Type Cu/Sn-Bi/Cu Solder Joints", *Journal of ELECTRONIC MATERIALS*, vol. 37, No. 11 (2008), pp.1721-1726
3. C. M. CHEN and C. C. HUANG, "Effects of Copper Doping on Microstructural Evolution in Eutectic SnBi Solder Stripes under Annealing and Current Stressing", *Journal of ELECTRONIC MATERIALS*, Vol. 36, No. 7 (2007), pp. 760-765
4. R. D. Hilty, N. E. Corman, H. Herrmann, "Electrostatic Fields and Current-Flow Impact on Whisker Growth", *IEEE TRANSACTIONS ON ELECTRONICS PACKAGING MANUFACTURING*, vol. 28, No. 1 (2005), pp. 75-84
5. Y.W.LIN, Y. S. Lai, "Tin whisker growth induced by high electron current density", *Journal of ELECTRONIC MATERIALS*, vol. 37, No. 1 (2008), pp.17-22
6. H. W. He, H. Y. Zhao, F. Guo and G. C. Xu, "Bi Layer Formation at the Anode Interface in Cu/Sn-58Bi/Cu Solder Joints with High Current Density", *J. Mater. Sci. Technol.*, Vol. 28, No. 1 (2012), pp. 46-52
7. H. W. He, G. C. Xu, F. Guo, "Effect of small amount of rare earth addition on electromigration in eutectic SnBi solder reaction couple", *Journal of Materials Science*, Vol. 44, (2009), pp. 2089-2096
8. H. W. He, G. C. Xu, F. Guo, "Electromigration-induced Bi-rich whisker growth in Cu/Sn-58Bi/Cu solder joints", *Journal of Materials Science*, Vol. 45, No. 2 (2010), pp.334-340
9. C. M. CHEN, L. T. CHEN, Y. S. LIN, "Electromigration-Induced Bi Segregation in Eutectic SnBi Solder Joint", *Journal of ELECTRONIC MATERIALS*, Vol. 36, No. 2 (2007), pp.168-172