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TECHNICAL PAPER

Modeling of interfacial intermetallic compounds in the application of very fine lead-free solder interconnections

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Abstract Intermetallic compounds (IMCs) are formed between lead-free solders and base metals during soldering processes. The morphology as well as the amount of the IMCs, in particular the interfacial IMCs, are important to mechanical performance of the solder joints in their service environment. This is especially the case in state-of-art ultrafine-pitch wafer-level packaging, in which solder joints could become as small as 50 μm in diameter or even less. However, research addressing growth kinetics of the IMCs in the existing literature has concentrated on fitting experimental data onto a simple parabolic growth equation, which cannot account for all the complicated physics involved in the process of IMC formation. There are a few models based on Fick's diffusion equations in the literature, which assume the growing IMC interface is planar. A combined thermodynamic–kinetic model has been derived from the relationships amongst some thermodynamic parameters; however, this model is only one dimension (1-D) in nature. 2-D models have also been proposed, e.g. an implicit boundary tracking method, and a phase field model. This paper reviews the modeling techniques in the literature for both the growth kinetics and morphology of the interfacial IMCs, under the context of lead-free soldering in very fine interconnections. The advantages and disadvantages of each method are discussed. Possible solutions to include the geometrical features of micro solder joints in the modeling of growth kinetics of interfacial IMC are presented.

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1 Introduction

The formation and growth of an IMC is a critical issue for the mechanical properties of solder joints and therefore the integrity of entire electronic products. Figure 1 shows the micrograph of a cross section of a Plastic Ball Grid Array (PBGA) flip chip joint (Sn–3.8Ag–0.7Cu) as well as typical materials present in each layer. The wafer level and board level metallizations in this case are electroless nickel and copper, respectively. The solder reaction with metallizations at the chip and substrate side in flip chip technology presents a dilemma. On one hand, a rapid solder reaction is required in order to achieve the joining of thousands of interconnections simultaneously. On the other hand, it is also desirable that the solder reactions stop immediately after joining, since the thin film Under Bump Metallization (UBM) is too thin to allow prolonged reaction. However, the manufacturing of a device usually requires these solder joints to endure several sequential reflow processes, in which the total period of a solder bump in the molten state can be several minutes (Tu et al. 2001). Hence, the solder-thin film reaction is a critical issue in electronic

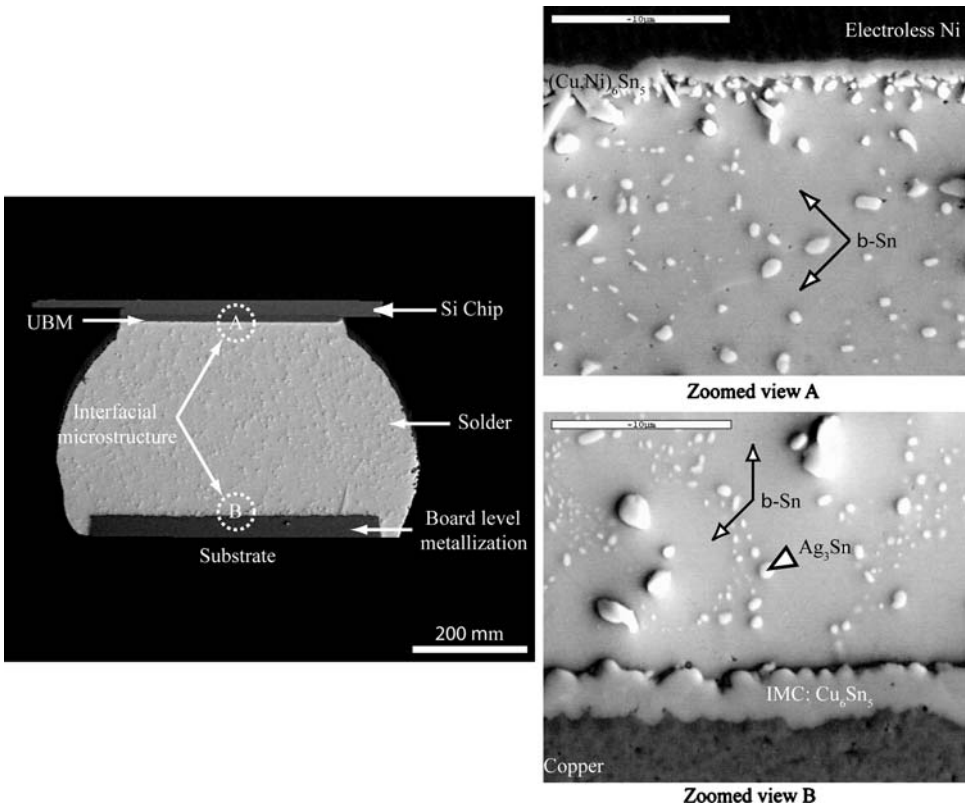

Fig. 1 A micrograph showing a cross section of Plastic Ball Grid Array (*PBGA*) flip chip joint (Sn–3.8Ag–0.7Cu) as well as typical materials present in each layer (courtesy of Dr. R. M. Horsley of Celestica)

manufacturing. As a result of the interactions between the solder and chip/board level metallizations, some intermetallic compounds (IMCs) form during the manufacturing processes and in-service life, e.g. $(Cu,Ni)_6Sn_5$ and Cu_6Sn_5 IMCs at the electroless nickel-solder and copper-solder interfaces respectively.

The miniaturization of microelectronic products requires the use of increasingly dense arrays of interconnects with increasingly fine solder joints. The miniaturization of the solder joints raises several issues that need to be addressed to enable the design of reliable packaging. In particular, when the solder joints are very small, i.e. with a diameter of 100 μm or even less, the morphology as well as the thickness of the interfacial IMC play an important role in controling the mechnical integrity of the joints. Recent experimental and modeling work (e.g. Huang et al. 2006; Ho et al. 2006; Huang et al. 2004, 2005; Kinyanjui et al. 2005) suggest that the solder joint size and geometry could influence kinetics of the interfacial IMC formation. Therefore, a high fidelity analytical tool, which is capable of describing the entire growth history of the IMC layers, is needed to accurately predict the relationship between the manufacturing process, long-term reliability and the features of the IMCs.

This paper reviews the current modeling techniques in the literature describing the growth kinetics of interfacial IMCs. The possible solutions to incorporate the geometrical information into the models for predicting the growth kinetics of the interfacial IMCs present in ultrafine lead free solder joints are also discussed. The paper begins with a critical review of the different modeling techniques in the literature and then discusses the possible solutions to incorporate geometrical parameters to accurately predict the growth kinetics of interfacial IMCs in very fine solder interconnections.

2 Modeling of IMC growth kinetics

Study of the growth kinetics of the interfacial IMCs is of great significance for the application of lead-free solders. For the fast growing electronics manufacturing industries, tedious studies of the growth kinetics of the interfacial IMCs for different lead-free solders/substrates combinations, chemical compositions, and process conditions by experiments are simply not affordable. As a result, different modeling techniques populate the literature for addressing the interfacial IMCs in solder applications. This section compiles and critically reviews those models.

2.1 Curve-fitting method

The curve-fitting method is commonly used in the existing literature (e.g. Yu et al. 2005; Kim et al. 2005). This

method uses IMC growth kinetics data obtained from a series of experiments to fit the following equation:

$$W = kt^n + A \tag{1}$$

where W is the thickness of IMC layer, k the growth rate constant, n the time exponent, t the reaction time and A the layer thickness at $t = 0$. The fitted growth rate constant k is then used to calculate the growth activation energy of the IMCs, which can be used to compare the diffusion mechanisms in different solder/substrate systems. This method is not sufficiently comprehensive to account for the complex underlying mechanisms of the IMC formation.

2.2 One and two dimensional analytical models

There are one dimensional (1-D) and two dimensional (2-D) analytical models, which are based on the Fick's diffusion equations and normally assume that:

(1) The growing IMC interface is planar;
(2) The intrinsic diffusion coefficients are constants within each individual phase;
(3) The volume change on the formation of the IMCs is negligible;
(4) Thermodynamic equilibrium is maintained at the growing IMC interfaces.

The moving interface positions can then be tracked using the mass balance equation at the interface ξ:

$$v_\xi = \frac{J_i^{\xi\alpha} - J_i^{\xi\beta}}{C_i^{\xi\alpha} - C_i^{\xi\beta}} \tag{2}$$

where v_ξ is the moving velocity of the interface, $C_i^{\xi\alpha}$, $C_i^{\xi\beta}$ are the concentrations of elements i in α and β phases, respectively, $J_i^{\xi\alpha}$, $J_i^{\xi\beta}$ are the corresponding fluxes. The 1-D analytical model is exemplified by Mei et al. (1992), Erickson et al. (1994), Lee et al. (1999), and Huh et al. (2004a, b). A study by Erickson et al. (1998) used a 2-D implicit boundary tracking method to model the solid-state IMC formation between a Sn–Pb solder and a porous substrate coating. To date, this model has not been extended to consider the solder joint size and geometry effects.

2.3 Energetics method

If the growth of the IMC is controlled by bulk diffusion only, the growth kinetics of the IMC can be described by:

$$\frac{dx}{dt} = \frac{k^2}{2x} \tag{3}$$

where x is the thickness of the growing IMC and k^2 is the temperature dependent reaction constant. For the case of 1-D growth of an IMC layer in a planar geometry, the heat flow, dH/dt, is directly proportional to the reaction rate, dx/dt:

$$\frac{dH}{dt} = \frac{A\rho\Delta H_r}{M}\frac{dx}{dt} \tag{4}$$

where M, ρ, and ΔH_r are the molar mass, density and the heat of reaction respectively, A is the interfacial area which is calculated from measurements of layer thickness. Integrating Eqs. (3) and (4), gives:

$$k^2 = \left(\frac{M}{A\rho\Delta H_r}\right)^2 \frac{H^2}{t} \tag{5}$$

It is possible to measure the heat flow, dH/dt, of the interfacial reaction by using differential scanning calorimetry (DSC). Thus, by first integrating the measurement of the heat flow as a function of time to obtain the integrated heat flow, H, and plotting H^2 versus time, the reaction constant, k^2, may be calculated (Chromik et al. 1996, 1997; Dreyer et al. 1996). This method is experimentally intensive, i.e. experiments must be carried out for every new solder-substrate system, and as such it is not efficient during the product design stage.

2.4 Dual-phase-lag model

The dual-phase-lag diffusion (DPLD) model was first developed for predicting the growth of the interfacial phase compound in metal matrix composites (Chen et al. 1999) and thin films (Chen et al. 2000). In view of the similarity between the kinetics of interfacial phase growth in MMC and solder joints, Chen et al. (2001) also applied the DPLD to modeling the IMC growth in solder joints, e.g. IMC growth in a 100Sn/Cu system at 170°C. Li et al. (2003) further applied the DPLD model to predict the growth of the interfacial IMC for the Sn–3.5Ag/Cu and Sn–3.5Ag–0.7Cu/Cu systems during reflow. This model can be used to explain some of the phenomena of the IMC growth in solder joints; however, it is a 1-D model in nature.

2.5 Combined thermodynamic and kinetic modeling

Combined thermodynamic and kinetic modeling provides useful information on the stabilities of phases, driving forces for chemical reactions, and growth rates of reaction products occurring in interconnections or thin-film structures during processing, testing, and in long-term use of electronic devices (Kivilahti 2002). Rönkä et al. (1998) assumed that interfacial IMC growth is diffusion controlled and proposed a 1-D combined thermodynamic–kinetic model based on the following three relationships:

(1) The relationship between the integrated diffusion coefficient and the IMC layer thickness;

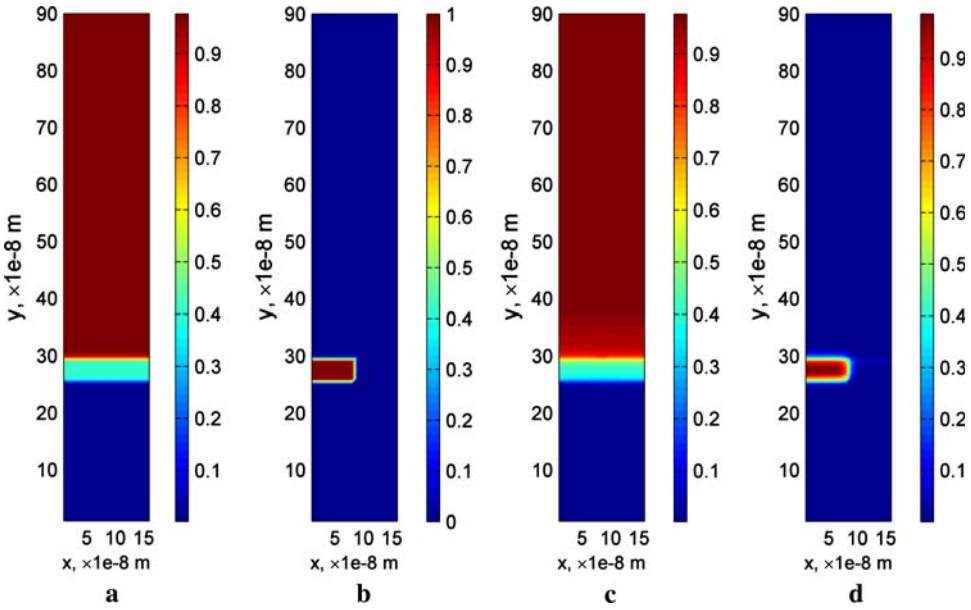

Fig. 2 Phase field modeling of tin-copper binary system with four initial Cu_6Sn_5 IMC grains (only two grains are simulated due to symmetry) **a** initial composition map; **b** initial order parameter map for one IMC grain; **c** composition map after 50 time steps (the same time step as in Huh et al. 2004 was used); and **d** order parameter map for the IMC grain after 50 time steps

(2) The relationship between the integrated and tracer diffusion coefficients;
(3) The relationship between the tracer diffusion coefficient and the driving force for IMC formation.

This is a general model that can be equally applied to other solder-substrate systems, as long as the thermodynamic data for the system are available. However, the disadvantage of this model is that experimental data with respect to the growth kinetics of the IMCs for a particular material system under consideration are required to retrieve constants for the model.

In theory, computational thermodynamics and kinetics tools such as Thermo-Calc (Sundman et al. 1985) and DICTRA (Borgenstram et al. 2000) can be used to simulate the growth kinetics of the interfacial IMCs. However, to the best knowledge of the authors, a comprehensive kinetic database specialized for lead-free solders is not yet available. In addition, there is no agreement yet on the diffusion mechanisms controlling the formation of the interfacial IMCs in different lead-free solders/substrates systems (Laurila et al. 2005). Ghosh (2001) has done some work using DICTRA to simulate the dissolution kinetics of Ag in molten solder, which is a process less complicated than the interfacial IMCs formation. It is worth noting that although some simple geometries can be assumed in DICTRA, the kinetics predicted by DICTRA are essentially 1-D.

Huang et al. (2006) have extended Rönkä's model to a 2-D scenario. 3-D combined thermodynamic and kinetic modeling is also possible with the latest development in the linkage between thermodynamic calculation software package and third party numerical computing tools (Huang et al. 2007).

2.6 Phase field models

Phase field models can simulate morphology and morphology evolution, which is an ideal technique for modeling the interfacial IMCs present in very fine lead-free solder interconnects, where the morphology as well as the thickness of the interfacial IMCs are of interest. Huh et al. (2004a, b) is the first one to use the phase field modeling technique to study the 2-D IMC growth during soldering reactions, although the original model was developed by Kim et al. (2004) for different material systems. The formulation of the free energy of the system in Huh's phase field model uses a "double obstacle potential" in contrast to a "double well potential".

In a phase field model, the effects of grain boundary diffusion, solder/IMC interface energy as well as the solder composition on the IMC growth can be incorporated into the phase field model. However, due to lack of information, such as thermodynamic and kinetic data for the material system, even creating a first input to the phase field model will require a lot of work when initializing a new calculation. In addition, some material data such as interfacial energy and mobilities are difficult or even impossible to measure, or find in the existing literature. Computation efficiency could be another challenge, in particular when the phase field model is coupled with the CALPHAD (CALculation of PHAse Diagrams) method or the scale of the simulation system is large, e.g. a larger number of IMC grains present in the system.

3 A geometrical issue

Both experimental and modeling results have suggested that solder bump size and geometries could influence the

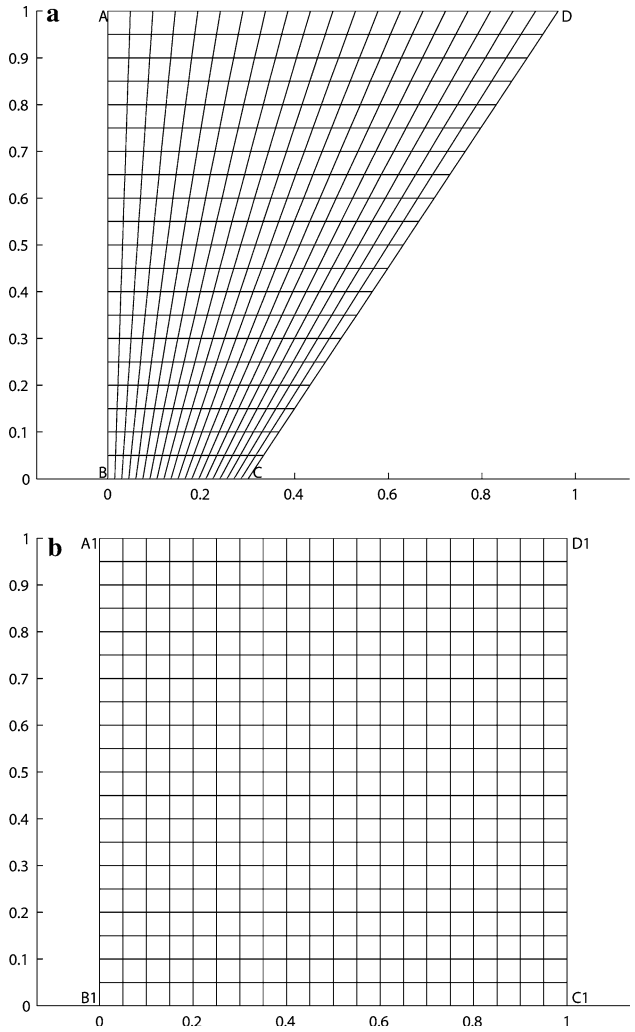

Fig. 3 **a** A trapezoidal domain ABCD with four corners at $(x, y) = (0, 0)$, $(b/2, 0)$, $(b/2+a, h)$, $(0, h)$, where $b = 0.6$, $a = 0.66$, $h = 1.0$. **b** After mapping using Eq. (8), ABCD transforms to a unit square A1B1C1D1

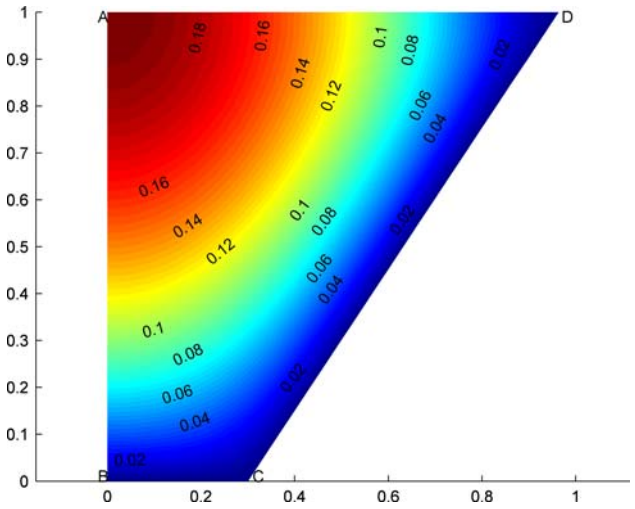

Fig. 4 Solution to the Poisson's equation, i.e. Eq. (6), with boundary conditions of Eq. (7) using standard finite difference method. The numbers in the figure are contour labels

growth kinetics and the morphology of the interfacial IMCs present in very fine lead-free solder interconnects. Looking at all the modeling techniques reviewed above, phase field models are the most promising and incorporate more physics for addressing growth kinetics of the interfacial IMCs. Using Huh's model, Fig. 2 presents the modeling results for the Tin–Copper binary system with four initial Cu_6Sn_5 IMC grains (only two grains are simulated due to symmetry). A majority of the phase field models (equations) are solved numerically by the finite difference method with a rectangular geometry. The geometries of interest in soldering are not rectangular (Huang and Conway 2007). Although it is possible to use the finite difference method to solve phase field equations on non-rectangular domains, the finite volume method or finite element methods are better alternatives to deal with complex geometries. A previous study (Huang and Conway 2007) compared the computational efficiency of using different numerical methods and computational tools for the same set of phase field equations of solidification.

In this paper, a different approach is proposed to use the finite difference method to solve partial differential equations on simple non-rectangular geometries ranging from trapezoidal to triangular domains. The basic idea is to construct a mapping between a rectangular region and the domain of interests. Depending on the complexity of the geometry, devising this mapping may be very difficult or simply not possible (Thompson et al. 1999). However, for simple geometries such as trapezoids and triangles, the mapping is possible. In contrast to rectangular geometries, trapezoids and triangles can represent, to some extent, the geometrical variation from the solder bump/substrate interface to the top of the solder bumps, which influences the kinetics of the inter-diffusion between the chemical elements in the solders and the substrates and thus the growth kinetics of the interfacial IMCs. After the mapping, the domain of interest is transformed to a rectangular geometry and then the transformed partial differential equations (with transformed boundary conditions) can be readily solved using the finite difference method.

To illustrate the idea, a simple equation, i.e. Poisson's equation is considered

$$-\nabla^2 u = 1 \tag{6}$$

on a trapezoidal domain ABCD is shown in Fig. 3a, subjected to the boundary conditions

$$\frac{\partial u}{\partial n} = 0 \text{ in } AB \text{ and } AD \text{ and } u = 0 \text{ in } BC \text{ and } CD \tag{7}$$

The four corners in the physical domain are located at $(x, y) = (0, 0)$, $(b/2, 0)$, $(b/2+a, h)$, $(0, h)$. A mapping

between the coordinates in the transformed coordinate system (ξ, η) on the unit square and (x, y) is

$$x = (b/2 + a\eta)\xi$$
$$y = h\eta \quad (8)$$

After mapping, the trapezoidal domain ABCD transforms to a unit square A1B1C1D1. The transformed partial differential equations are then solved by a standard finite difference method and the result is shown in Fig. 4.

4 Summary

This paper discusses the advantages and disadvantages of different modeling techniques in the literature on the growth kinetics of interfacial IMCs in lead-free soldering applications. Phase field models are recommended for the prediction of the growth kinetics of the interfacial IMCs presented in very fine lead-free solder interconnects, where the morphology as well as the thickness of the IMCs is of significance. A mapping method has been proposed such that phase field equations on domains of trapezoidal or triangular shapes can be solved by standard finite difference method.

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References

Borgenstam A, Engström A, Höglund L, Ågren J (2000) DICTRA, a tool for simulation of diffusional transformations in alloys. J Phase Equilibria 21(3):269–280

Chen JK, Beraun JE, Tzou DY (1999) A dual-phase-lag diffusion model for interfacial layer growth in metal matrix composites. J Mater Sci 34(24):6183–6187

Chen JK, Beraun JE, Tzou DY (2000) A dual-phase-lag diffusion model for predicting thin film growth. Semiconductor Sci Technol 15(3):235–241

Chen JK, Beraun JE, Tzou DY (2001) A dual-phase-lag diffusion model for predicting intermetallic compound layer growth in solder joints. J Electron Packag 123(1):52–57

Chromik RR, Cotts EJ (1996) A Study of the kinetics and energetics of solid state reactions in Pd/Sn diffusion couples. In: Materials research society symposium proceedings, vol 398, pp 307–312

Chromik RR, Cotts EJ (1997) Thermodynamic and kinetic study of phase transformations in solder/metal systems. In: Materials research society symposium proceedings, vol 445, pp 31–36

Dreyer KF, Neils WK, Chromik RR, Grosman D, Cotts EJ (1996) Calorimetric study of the energetics and kinetics of interdiffusion in Cu/Cu6Sn5 thin film diffusion couples. In: Materials research society symposium proceedings, vol 398, pp 313–318

Erickson KL, Hopkins PL, Vianco PT (1994) Solid-state intermetallic compound growth between copper and high-temperature, tin-rich solders-Part II—modeling. J Electron Mater 23(8):729–734

Erickson KL, Hopkins PL, Vianco PT (1998) Modeling the solid-state reaction between Sn–Pb solder and a porous substrate coating. J Electron Mater 27(11):1177–1192

Ghosh G (2001) Dissolution and interfacial reactions of thin-film Ti/Ni/Ag metallizations in solder joints. Acta Mater 49:2609–2624

Ho CE, Liu YW, Yang SC, Kao CR, Jiang DS (2006) Effects of limited Cu supply on soldering reactions between SnAgCu and Ni. J Electron Mater 35(5):1017–1024

Huang ZH, Conway PP (2007) A comparative study of numerical methods and computational tools for phase field equations of solidification. In: 2007 TMS Annual Meeting and Exhibition. Advances in Computational Materials Science and Engineering Methods, pp 1–9

Huang ZH, Conway PP, Jung E, Thomson RC, Liu CQ, Loeher T, Minkus M (2006) Reliability issues in Pb-free solder joint miniaturization. J Electron Mater 35(9):1761–1772

Huang ZH, Conway PP, Liu CQ, Thomson RC (2004) The effect of microstructural and geometrical features on the reliability of ultrafine flip chip microsolder joints. J Electron Mater 33(19):1227–1235

Huang ZH, Conway PP, Liu CQ, Thomson RC (2005) Effect of solder bump geometry on the microstructure of Sn-3.5 wt% Ag on electroless nickel immersion gold during solder dipping. J Mater Res 20(3):649–658

Huang ZH, Conway PP, Thomson RC, Dinsdale AT, Robinson JAJ (2008) A computational interface for thermodynamic calculations software MTDATA. CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 32(1):129–134. doi: 10.1016/j.calphad.2007.07.003

Huh JY, Han SU, Park CY (2004) Effect of bismuth on the growth kinetics of intermetallic compounds in Sn-3.5Ag solder joints—a growth kinetic model. Metals Mater Int 10(2):123–131

Huh JY, Hong KK, Kim YB, Kim KT (2004) Phase field simulations of intermetallic compound growth during soldering reactions. J Electron Mater 33(10):1161–1170

Kim DG, Jung SB (2005) Interfacial reactions and growth kinetics for intermetallic compound layer between In-48Sn solder and bare Cu substrate. J Alloys Compounds 386(1–2):151–156

Kim SG, Kim WT, Suzuki T, Ode M (2004) Phase-field modeling of eutectic solidification. J Crystal Growth 261(1):135–158

Kinyanjui R, Lehman LP, Zavalij L, Cotts E (2005) Effect of sample siye on the solidification temperature and microstructure of SnAgCu near eutectic alloys. J Mater Res 20(11):2914–2918

Kivilahti JK (2002) The chemical modeling of electronic materials and interconnections. JOM 54(12):52–57

Laurila T, Vuorinen V, Kivilahti JK (2005) Interfacial reactions between lead-free solders and common base materials. Mater Sci Eng R-Rep 49(1–2):1–60

Lee YG, Duh JG (1999) Interfacial morphology and concentration profile in the unleaded solder/Cu joint assembly. J Mater Sci Mater Electron 10(1):33–43

Li GY, Chen BL (2003) Formation and growth kinetics of interfacial intermetallics in Pb-free solder joint. IEEE Trans Components Packag Technol 26(3):651–658

Mei Z, Sunwoo AJ, Morris JW (1992) Analysis of low-temperature intermetallic growth in copper-tin diffusion couples. Metall Mater Trans A 23(3):857–864

Rönkä KJ, Van Loo FJJ, Kivilahti JK (1998) A diffusion-kinetic model for predicting solder/conductor interactions in high density interconnections. Metall Mater Trans A 29(12):2951–2956

Sundman B, Jansson B, Andersson JO (1985) The thermo-calc databank system. CALPHAD 9(2):153–190

Thompson JF, Soni BK, Weatherill NP (1999) Handbook of grid generation. CRC Press, London

Tu KN, Zeng K (2001) Tin-lead (SnPb) solder reaction in flip chip technology. Mater Sci Eng R 34(1):1–58

Yu DQ, Wu CML, Law CMT, Wang L, Lai JKL (2005) Intermetallic compounds growth between Sn–3.5Ag lead-free solder and Cu substrate by dipping method. J Alloys Compounds 392(1–2):192–199