Investigation of Sn grain growth in solder joints by numerical simulations

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Abstract—The microstructure of the solder joint determines the basic quality and reliability parameters of the solder joints, like the electrical- and thermal-conductivity, the mechanical parameters, the thermal stability, the corrosion resistance, etc. So, investigating the solder joints' microstructure is an important aspect of the soldering technology. The basic method of microstructural investigations is the optical observation of 2D cross-sections of the solder joints, which can be misleading since we make conclusions from a 3D structure according to a 2D view. Therefore, our aim is to develop a 3D numerical simulation environment that can calculate the Sn grain formation during the solidification of the solder joint. Our method is based on the decentred octahedron growth algorithm, which is a type of cellular automaton (CA) model, used to predict microstructure during solidification. The dendritic network in each cell is covered by a polyhedron envelope, while the growing envelopes during cooling capture neighbouring cells, resulting in grain growth.

Keywords—grain growth, solder joint, reflow, numerical simulation, FDM

I. INTRODUCTION

Among the lead-free solders the SnAgCu (SAC, Sn >95%) is one of the most promising substitutes for conventional Sn–Pb solder. The intermetallic (IMC) layer thickness, the size of the Sn grains (β-Sn), the amount and the size of the dispersed Cu6Sn5 and Ag3Sn IMC particles in the solder bulk, so generally, the microstructure of the solder joint determines the basic quality and reliability parameters of the solder joints. The microstructure affects the electrical- and thermal-conductivity, the mechanical parameters, the thermal stability, the corrosion resistance, the Sn whisker and electrochemical migration susceptibility [1]. The most recent solution to improve the microstructure of the solder joints is adding reinforcement particles into the solder alloys. The particles are usually nano-sized ceramics like, TiO2, ZrO2, Al2O3, Fe2O3, Si3Ni4, SiC, La2O3, etc. [2] in 0.05 – 2 wt%, resulting in „nano-composite" or simply "composite" solder joints. Three methods can be used for preparing composite solders: the addition of the nano-particles (NPs) during alloying; the mixing of the NPs into the solder paste (mostly used); and the powder metallurgy, which means the mixing of the NPs and solder powder before the paste preparation. The ceramic NPs are not soluble in the Sn solders, so they incorporate at the Sn and IMC grain

boundaries, where they promote heterogeneous nucleation. This results in the suppression of grain growth (at all phases) and decreases dislocation motions [3]. The finer microstructure can improve the solder joints' mechanical properties (shear force, yield strength, microhardness, etc.), with only some Kelvin of change in the melting temperature of the alloy.

So, investigating the microstructure and grain growth mechanism during the solidification are important aspects of the quality and reliability forecast of the joints. The basic method of investigation is the 2D cross-sectioning of the solder joints and observing the microstructure by optical or scanning electron microscopy (SEM). Although a well-established method, making conclusions of a 3D structure according to a 2D view can be misleading. Nowadays, the increasing computational capacities allow us to investigate by numerical simulations, which can offer further novel and interesting aspects of the topic.

II. NANO-COMPOSITE SOLDER

A. Solidification of SAC solder

During the solidification of SnAgCu solder joints the nucleation of liquid Sn requires considerable undercooling (10-20 ºC or even more below the liquidus line) that leads to rapid dendritic growth to form a polycrystalline microstructure Once the Sn solidification started, the high release rate of latent heat causes the solder to heat up, eventually suppressing further Sn nucleation in the volume, but the growth of already established grains will continue. Usually, the nucleation undercooling of the melt increases as the size decreases or the cooling rate increases [4]-[7].

Because of large undecooling during solidification, IMCs may be formed even before the β-Sn phase with rod-like shape for Cu6Sn5 and plate- or needle-like for Ag3Sn throughout the melt. Lower cooling rate promotes this behaviour by allowing the diffusion and aggregation of solute atoms, especially for Cu6Sn5 grains. These tend to grow onto pure copper pads at the root of the joints. This layer also can provide additional nucleation sites for the upcoming Sn dendrite growth [7]-[10]. This can even result in the abnormal case, where the lower cooling rate yields the smaller grain size.

The Sn grain structure has two distinct variant observed in SAC solidification studies as they appear on polished cross-sections under polarised light and on electron backscatter diffraction (EBSD) images, as seen on Fig. 1 and Fig. 2. The interlaced type appears as a patched texture containing many small, seemingly random oriented grains, while the beach ball type shows few large Sn grains that are cyclically twinned with nominally 60° rotations about the [100] axis [4][5]. It is likely that these large grains appear as polycrystalline macrograins consist of smaller grains with very similar orientation [8]. Generally it is expected that the Sn grain structure is as a mixture of the two [11].

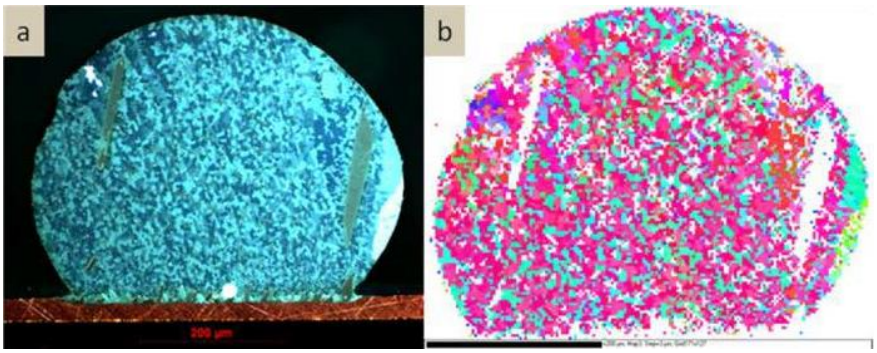

Fig. 1. (a) Cross polarized image of SAC 205 on Cu substrate showing interlaced structure; (b) EBSD map of the same sample [6].

Fig. 2. (a) Cross polarized image of SAC 205 on Cu substrate showing beach ball cycling twinning; (b) EBSD map of the same sample [6]

B. *Effect of additional NPs*

Studies have shown that the microstructure of the solder can be improved by adding appropriate second phase particles. This method stand as an economically viable process that produces composite solder pastes. The finer Sn and IMC grains (Fig. 3) generally result in favourable solder joint properties like increased microhardness, tensile and yield strength, also decrease the thermal expansion coefficient. On the negative side only the minor increase of the liquidus temperature is known currently [1]-[3].

The mechanism of action is complex and diverse for NPs. When present in the polycrystalline matrix, they can prevent dislocation motion, strengthen against creep deformation. Similarly, they act a diffusion barrier, prohibiting IMC growth. Large IMCs can locally accumulate strain at the grain boundaries, and they are also brittle, lowering the mechanical strength altogether. Furthermore, NPs provide additional nucleation sites that provide finer grain structure during solidification [2][3][12]. It is also likely that they can generally suppress grain growth by boundary pinning, decreasing the growth speed locally [12]-[14]. It was additionally observed that TiO_2 particles can bond with Sn atoms at the grain boundaries, effectively preventing solder joint oxidation [1].

III. GRAIN GROWTH SIMULATION

The two main types of metallic grain growth simulations are the deterministic and stochastic methods, capable to calculate grain structure development and dendrite growth during either solidification or heat treatment (grain coarsening). The typical example of the first type is the phase field method that handles curved grain interfaces with smoothly varying phase variables. It is an exact physical model that requires enormous computation resource to solve over large domains, and many types are constricted to 2D [13]. On the other hand, stochastic methods are more like parametric behavioural models that also include the necessary deterministic mechanisms. The cellular automaton (CA) based models are stochastic type and

the basic technique was introduced in 1993 [15]. They require less computation power, thus capable to handle large 3D sample size (mm and beyond) [16]-[19].

A. The basics of the CA model

Our aim is to develop a 3D numerical simulation environment that can calculate the Sn grain formation during the solidification of the solder joint in the function of the cooling gradients and the amount and distribution of the NPs in the solder bulk. Our method is based on the 3D decentred octahedron growth algorithm, a type of cellular automaton (CA) model used to predict microstructure during solidification [16]. This approach covers nucleation and grain growth on a 3D grid, containing cubic cells. The possible nucleation sites are randomly selected and a critical undercooling value is assigned to them during the initialisation process. This critical value needs to be reached to nucleate the cell. It is very important that these values have a normal distribution, where the mean value and the deviation are parameters. When properly set, they guarantee finer grain structure with larger cooling rates as it resulted in larger nucleation rate. After nucleation, the dendritic network in each cell is assumed to be developed as an octahedral envelope with random orientation (Fig 4.). Depending on the local cooling rate, the size of each envelope is calculated in every time step, while the growing envelopes capture neighbouring cells eventually. A new envelope is initialised in the captured cell, inheriting the orientation of the capturing envelope, resulting in grain growth.

Modifications and extensions

According to the literature, below we summarised the necessary modifications and extensions to the basic algorithm to properly represent Sn grain growth in composite solders.

- The original CA model and its later variants are used to model metals with FCC (face centred cubic) lattice. These type of metals have the <100> preferred dendritic orientation [20]. However, Sn is BCT (body centred tetragonal) with the <110> preferred orientation [21]. Following the same logic of polyhedral crystal growth, the dendrite envelope should be modified from octahedron to cuboctahedron (Fig. 5.) [22].
- The basic CA algorithm is adapted to the interlaced growth mechanic. The beach ball like behaviour should be implemented through a specialised cyclically twinned nucleus [11].
- Effect of NPs, namely additional nucleation sites and prohibited grain growth should be implemented. This will be shown in the next sections.
- Effect of IMCs, namely the additional nucleation sites above copper pads should be implemented. It is also seems possible for very large plate like IMCs to stand as an obstacle against the Sn grain, promoting boundary formation.

- Because of the extensive latent heat release during solidification, the CA model should be coupled to the heat equation. This can done with a heat source term that proportional with the change rate of the liquid fraction [23].

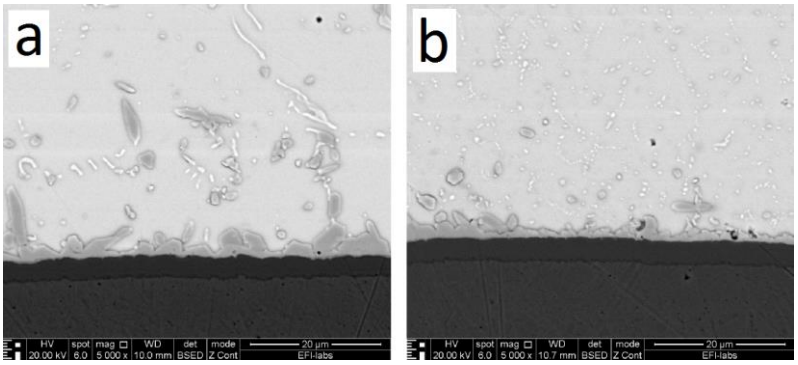

Fig. 3. (a) SEM image of the IMC structure of SAC 305 on Cu pad; (b) refined IMC structure due to TiO2 NPs.

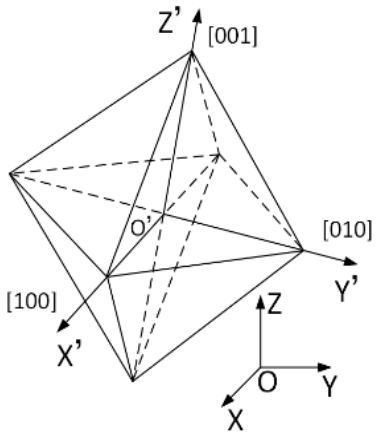

Fig. 4. Oriented local octahedron (O', X', Y', Z') is shown in the global system (O, X, Y, Z).

B. Simulation parameters

The simulation project was realised in MATLAB environment. We used 220 ºC liquidus temperature, 10 ºC mean critical undercooling on a 40x40x40 uniform grid with 5 μm resolution (64000 cells total). Each cell had a 0.3% chance to be initialised as possible nucleation site, thus 190 was the expected value.

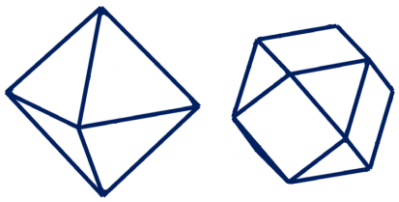

Fig. 5. Comparison of the octahedron (left) and the cuboctahedron (right) envelopes.

The grain growth speeds in pure metals are very high as they even reach the order of tens of cm/s [24]. However, solidification studies for alloys typically calculate polynomials in the order of few mm/s with comparable undercooling [16]-[18]. Relevant data for SAC alloy are scarce, and as an approximation we used the polynomial given for pure Sn in [24] decreased by two orders of magnitude as:

$$\nu = 0.022 \cdot (\Delta T)^{1.81} \qquad (1)$$

where ν [mm/s] is the dendrite growth speed and ΔT [K] is the undercooling.

The proper order of magnitude for the deviation of the critical undercooling depends on the growth speed. It must be carefully selected to ensure the typical cooling rates (0.1-1-10 ºC/s) have the expected effect. We used 0.1 ºC and the obtained results with uniform cooling, yet without NPs, are shown below (Fig. 6). For each grain the angle between the local Z' axis ([001] of the local octahedron) and the global Z axis are shown. Because of the symmetry, it is in the range of 0-90º. The grain structures are shown after 100% solidification. It can be observed in Table 1 that the nucleation ratio (NR%, ratio of the possible and actual sites) and thus the total grain number (TG#) increased with higher cooling rates. The consequence is decreased grain size and finer grain structure.

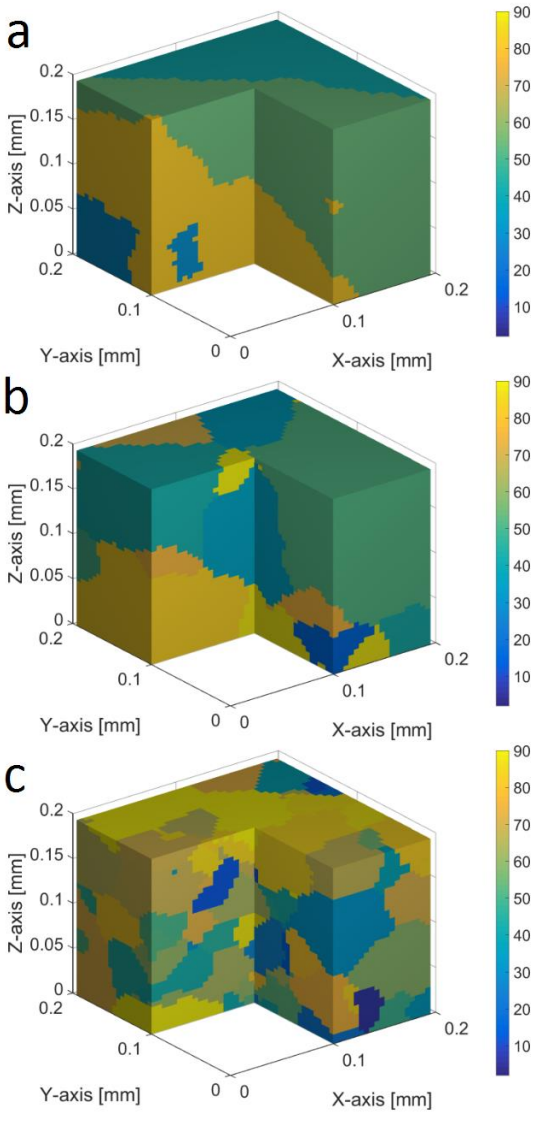

Fig. 6. Comparison of the grain structures with different cooling rates: (a) 0.1 ºC/s - 2.4 NR%, 5 TG#; (b) 1 ºC/s - 9.5 NR%, 18 TG#; (c) 10 ºC/s - 81 NR%, 156 TG#. The colour map means the angle of the local [001] direction. The corner was cut off to show inner region.

C. *Modelling the effetc of NPs*

We have experimented with the basic model to find the optimal way (with minimal changes) to show the response to NPs. We found that the implementation can be done by organised parameter modification. Two independent effects were distinguished: pinning and nucleation. Each one is capable to promote finer grain structure, which means larger TG# after solidification. During real experiments both effect appear simultaneously.

The pinning effect (P-effect) means prohibited grain growth. It was modelled by decreasing the grain growth speed proportionally to the local distribution of NPs. It can provide finer grain structure by saving possible nucleation site from capturing early by other grains that already grow. The efficiency depends on the cooling rate. After decreasing the speed uniformly to 50% or the original value in the whole domain, the obtained results are listed in Table 1. By comparing to the original values, it seems that with already high NR% the decreased growth speed had less effect relatively, but gives more additional grain on absolute scale. The pinning effect increased both the NR% and TG#.

The nucleation effect (N-effect) means additional possible nucleation sites. It was modelled by selecting additional sites with a probability that proportional to the local distribution of NPs. More possible sites straightforwardly mean finer grain structure using the same conditions. After using 0.3% uniform probability to initialise additional possible nucleation sites (expectedly doubling them) we got the results listed in Table 1. It can be seen that the NR% mostly decreased or remained similar, meanwhile the TG# increased with the additional sites compared to the original values. The effect was especially significant at 10 ºC/s cooling rate, where the nucleation was already prominent. Just adding more possible nucleation sites does not generate significant changes until the dynamic temperature field does not assist to the nucleation process.

TABLE I. SUMMARISED GRAIN GROWTH RESULTS

Cooling rate	**Basic**		**P-effect**		**N-effect**	
	NR %	***TG #***	***NR %***	***TG #***	***NR %***	***TG #***
0.1 ºC/s	2.4	5	5.2	10	2.7	10
1 ºC/s	9.5	18	19.1	36	6	24
10	81	15	97.4	18	68.8	24

Cooling rate	Basic		P-effect		N-effect	
	NR %	***TG #***	***NR %***	***TG #***	***NR %***	***TG #***
ºC/s		6		9		5

IV. CONCLUSION

Sn grain growth in SAC alloy was modelled with the CA method. We were able to reproduce the effect of NPs during solidification resulted in finer grain structure. Further development will incorporate other main features of Sn grain growth as pointed out in the literature. This also means full coupling to the dynamic temperature field via the latent heat of solidification. Our long-term goal is to create a numerical model that can be used as a tool for process optimisation.

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