Discrete Phase Model (DPM) study of nano-reinforced Lead Free Solder Sn-3.0Ag-0.5Cu (SAC305)

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Abstract. This paper presents a preliminary study of the interaction between two models of numerical simulation namely volume of fluid (VOF) and discrete phase model (DPM). The multiphase-DPM model is capable of tracking the trajectory of the TiO\textsubscript{2} nanoparticles that has been doped in the lead free solder Sn-3.0Ag-0.5Cu (SAC305). The current model was developed based on passive surface mount component 01005 capacitor that undergoes conventional reflow process. The trajectory of the nanoparticles at 0.01, 0.05 and 0.15wt\% in the molten solder is shown in the flow front of the wetted molten solder. At 0.05wt\% of nanoparticles, good dispersion of nanoparticles, pressure distribution and wetting time was found. The difference in wetting time are about 3.76\% and 0.46\% for 0.05wt\% and 0.15wt\% compared to 0.01wt\% nanoparticle. The trajectory of the nanoparticles are shown to move along with the wetting formation of the molten solder. The pressure distribution and velocity vector of the different weight percentage of nanoparticles are also be studied. Higher pressure distribution is found at the capacitor area and intermetallic compound (IMC) region. The higher pressure distribution projected to reduce the micro void formation and optimize the reliability of the solder joint.

1. Introduction
Surface mount technology have allowed diversification in optimizing and sustaining the reliability of the integrated circuit (IC) package and miniaturization of passive and active components. In order to improve the reliability and performance of the electronic assembly, various types of nanoparticles have been used as the reinforced material doped in the molten solder [1]. The presence of foreign element in lead free solder such as aluminum oxide (Al\textsubscript{2}O\textsubscript{3}), nickle oxide (NiO), and titanium dioxide (TiO\textsubscript{2}) have changed the mechanical properties and microstructure of the lead free solder [2,3,4]. Y. Tang et al found that the hardness value of reinforced solder with TiO\textsubscript{2} nanoparticles increases by 34\% [5] and wettability of the solder material was improved at 0.05-0.1 wt\% nanoparticles [6].
In the fluid modelling, finite volume (FVM) based model has been shown to have vast capability of modelling fluid with high accuracy [7]. This model only have limitation of solving continuous flow and limited to tracking nanoparticle movement. From literature, various study on the DPM has been introduced mainly in fluidized beds that computes gas-solid fluidization as a mean to track the particles trajectory [8]. Additionally, the ability of DPM model to simulate and track particles has also been study by S. Rashidi et al in convective AL2O3–water nanofluid [9], N. Kharoua, et al in prediction of Black Powder distribution [10] and S. Lin et al in particle gasification [11].

Previous studies that have been conducted in the use of DPM model show the capability of particle tracking but have limitation in the study of coupling between both multiphase and discrete phase method. In this study, a two way interaction of multiphase and discrete phase model (DPM) is developed to track and analyse the trajectory of the nanoparticles that is being doped in the lead free solder Sn-3.0Ag-0.5Cu (SAC305).

2. Method

The numerical model used in this study is based on Navier-Stokes equation that involve conservation of mass and momentum:

Continuity equation:
\[
\frac{\partial \rho}{\partial t} + \nabla (\rho \mathbf{u}) = 0
\]  

Energy equation:
\[
\rho C_p \frac{\partial T}{\partial t} + \nabla (\rho \mathbf{u} T) = \nabla (k \nabla T) + \Phi
\]  

Momentum equation:
\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \tau + \rho g
\]

in which, \( \rho \) denotes the density of the fluid, \( \mathbf{u} \) is the velocity, \( \tau \) is the shear stress and gravity, \( g = -9.81 \) m/s.

The model is based on two phase interactions of SAC305 and air. Both phases are distinguished by the volume of fraction (VOF) in the range 0 to 1 with \( f = 1 \) indicating the presence of SAC 305 solder as described below,

VOF transport equation:
\[
\frac{\partial f}{\partial t} + \nabla (f \mathbf{u}) = 0
\]

The trajectory and tracking of the nanoparticles in the fluid are associated with the mass and other forces exerted on each of the nanoparticles as given by:

Particle force balance:
\[
\frac{\partial \mathbf{u}_p}{\partial t} = F_D (\mathbf{u} - \mathbf{u}_p) + g \frac{(\rho_p - \rho)}{\rho_p} + F_x
\]

where \( F_D (\mathbf{u} - \mathbf{u}_p) \) is the drag force associated with the velocity of fluid and particles, \( \mu \) is the molecular viscosity of the fluid, \( \rho_p \) is particle density and \( d_p \) is the particle diameter.

Additional force, \( F_x \) is related to the mass, acceleration and pressure gradient in the fluid based on the consideration that \( \rho >> \rho_p \).

\[
F_x = \frac{\rho}{\rho_p} \mathbf{u}_p (\frac{\partial \mathbf{u}}{\partial t})
\]
The dispersion and movement of the particle in a fluid is described by the Brownian motion of the particles. The interaction of the particle with the fluid medium is associated with the Brownian force, $F_B$ as:

$$F_B = \frac{\xi}{\eta} \sqrt{\frac{\pi D_0}{\Delta t}}$$

(7)

Additionally, the force that takes into consideration the effect nanoparticle sizes in terms of the interaction of lift, shear and drag exerted on each of the particle is the Saffman’s lift force. Due to the low particle Reynolds number, this force always acts upward.

Saffman’s lift force:

$$F_L = \frac{2Kv^{1/2}}{\rho d_k}\left(\frac{u - u_p}{d_{ij}}\right)^{1/4}d_{ik}$$

(8)

where, $v$ = kinematic viscosity, $K = 2.594$, constant, and $d_{ij}, d_{ik}, d_{ki} = \text{deformation tensor}$.

The nanoparticle is expected to move along with the formation of the wetting which shows two way interaction of the multiphase-DPM.

3. Numerical Simulation Setup

The environment of conventional reflow process is replicated in Ansys FLUENT using two way interactions of multiphase VOF and DPM model. A 3-dimensional model of a 01005 capacitor was constructed and will undergo a two-way interactions with the mixed solder paste. The discrete particle phase will enable precise prediction of the trajectory nanoparticles. The schematic diagram and mesh model of the printed circuit board (PCB) and 01005 capacitor are represented in Figure 1. The mesh developed for the current model is based on tetrahedrons mesh. A 3-dimensional model is developed to mimic real PCB and 01005 capacitor as shown in Table 2.

The Sn-3.0Ag-0.5Cu (SAC305) is used as the molten solder and nanoparticles doped with TiO2 nanoparticles and the properties are tabulated in Table 2. The SAC305 is initially patched into the mesh grid with the volume fraction of 1 to simulate real industry environment. The nanoparticles with weight percentages of 0.01, 0.05, and 0.15wt% are doped in the molten solder.

The solver used to solve coupling of both pressure and velocity in this model is Semi-Implicit Method (SIMPLE) algorithm scheme. This numerical solver is used to obtain high accuracy result.

Figure 1. Schematic diagram of the (a) PCB model with mounted 01005 capacitor, and (b) (c) 01005 capacitor.
Table 1. Dimension of the FR4-PCB and 01005 capacitor.

| DIMENSIONS (MM)               |
|------------------------------|
| FR4-PCB 255.0 x 178.0 x 2.0 |
| 01005 Capacitor 0.4 x 0.2 x 0.2 |

Table 2. SAC305 solder and TiO2 nanoparticle properties

| Properties SAC305                      |
|----------------------------------------|
| Density, \( p \) 7380 kg/m\(^3\)      |
| Specific heat capacity, \( C_p \) 230 J kg\(^{-1}\) K |
| Thermal Conductivity 58 Wm/K           |
| Viscosity 0.002 kg/ms                  |
| Standard state enthalpy 0.04 J/mol      |

| Properties TiO\(_2\)                  |
|----------------------------------------|
| Density, \( p \) 4250 kg/m\(^3\)      |
| Specific heat capacity, \( C_p \) 686 J kg\(^{-1}\) K |
| Thermal Conductivity 8.95 Wm/K         |
| Diameter, \( d \) \approx 20 nm        |

4. Result and Discussion

4.1. Flow Front Pattern

Figure 2 presents the flow front of the wetting molten solder with the trajectory of the nanoparticles at different weight percentages of 0.01, 0.05, and 0.15wt%. From the flow front, it can be shown that the nanoparticles trajectory are dispersed according to the motion of the wetting molten solder. The dispersion of the nanoparticles at some extent varies due to different concentration of nanoparticles present in the molten solder. At 0.01wt% of nanoparticles, the lowest trajectory and dispersion of the nanoparticles were found. This is due to the small amount of nanoparticles being injected in the molten solder. Better dispersion of the nanoparticles in the wetted molten solder is given by 0.05wt% of nanoparticles compared to 0.01wt% and 0.15wt%. At 0.15wt% of nanoparticles, the trajectory of the nanoparticles tends to accumulate at the upper layer of the molten solder. The dispersion of the nanoparticles at the upper layer was influenced by the buoyancy effect and density due to the density of the nanoparticles are much smaller compared to SAC305. The randomness and instability of the dispersion of nanoparticle will reduce the strength and the reliability of the solder joint. As studied previously by T. Laurila et al, failure result was found showing in drop test analysis for the case of more than 0.1wt% addition of reinforcement material into the SAC solder [12].

![Figure 2. The flow front of the different weight percentage of nanoparticles.](image)

The distribution of pressure and velocity in the wetted molten solder is depicted in Figure 3. The trajectory of the velocity vector for 0.15wt% is higher compared to 0.05wt% and 0.01wt% due to the higher concentration of the nanoparticle presents in the molten solder as in Figure 3. From Figure 3, the highest distribution of pressure is shown at the bottom of the PCB pad and side terminal of the 01005 capacitor. This due to the mechanism of the formation wetted solder which associates with
surface tension, since higher surface tension means more wetting and more exerted force, then more pressure. At 0.05wt% show higher pressure distribution compared to 0.01wt% and 0.05wt%. During the instantaneous nanoparticles dispersion in the molten solder, the nanoparticles that are present at the high pressure contour have the possibility to inhibit the formation of micro-voids. The trajectory of the nanoparticles typically at the higher pressure region have the lower possibility of the micro-voids formation. This was proven in a research by A. Abas et al [13] and M. H.H Ishak et. As the size of the particles in the nano-scale, the nanoparticles are exerted velocity same as the al [14] which found that the possibility of void formation is lower at higher pressure distribution.

\[\text{Figure 3. Pressure distribution and velocity vector at different weight percentage of nanoparticles.}\]

4.2. Wetting Time

Figure 4 depicted the plot of wetting time against wetting percentage for different weight percentage of the nanoparticles. At higher weight percentage of the nanoparticles, the wetting time increases. The addition of more particles seems to increase the surface that subsequently promotes the wettability of the mixed SAC solder. At 20% of wetting percentage, the time taken for each case is 1.823s, 1.712s, and 1.515s for 0.01, 0.05 and 0.15wt% respectively. Additionally, at 80% wetting percentage, the wetting time for 0.01, 0.05 and 0.15wt% are 2.820s, 2.926s, and 2.833s. There occurs a slight difference about 3.76% and 0.46% of wetting time for 0.05wt% and 0.15wt% compared to 0.01wt% nanoparticles. This as previously mentioned is due to the alteration of the current surface leading to an improved wetting capability.
5. Conclusion

This paper studies the dispersion of the discrete nanoparticles doped in SAC305 molten solder. The model was developed based on two way interactions of the multiphase-DPM model finite volume based simulation. The trajectory of the nanoparticles in the wetted molten solder is being tracked based on the flow front pattern of the simulation at different weight percentage of nanoparticles at 0.01, 0.05 and 0.15wt%. The nanoparticles trajectory for 0.05wt% is shown to have the best dispersion in comparison other nanoparticles percentages. The current model also shows the pressure distribution and velocity vector of the nanoparticles due to its direct effect on the reliability and strength of the solder joint. The study also found high pressure distribution at the vicinity of the component and intermetallic compound (IMC) region. The high pressure distribution is expected to reduce micro void formation. The addition of nanoparticles found slight increment in the wetting time as weight percentages of nanoparticles are increased.

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