EXPERIMENT AND SIMULATION REFLOW PROCESS OF PDMS MATERIAL

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DECLARATION

This work has not previously been accepted in substance for any degree and is not being concurrently submitted in candidature for any degree.

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ABSTRAK

Pembungkusan elektronik memainkan peranan yang tidak kurang pentingnya dalam industri elektronik. Komponen elektronik telah mengalami perubahan daripada komponen yang tidak regang kepada komponen yang elastik. PDMS biasanya merupakan bahan untuk menghasilkan komponen elektronik yang elastik. Akan tetapi, soldier yang diperbuat daripada PDMS menjalinkan perjalanan elektrik yang kurang memuaskan. Hal in demikian kerana bahan pengisi (perak) tidak menyambung dengan rapat. Oleh sebab itu, pertukaran pengisi daripada powder perak kepada serpihan perak dilakukan. Simulasi dijalankan untuk memerhati distribusi serpihan perak. Bahan pengisi soldier akan dianggap sebagai partikel and disimulasi menggunakan interaksi antara VOF dan DPM. Peratusan berat perak yang berlainan dipilih untuk dijalankan simulasi. Peratusan berat ini akan mempunyai kesan kepada distribusi, masa untuk basah, halaju dan tekanan. Masa untuk basah akan tambah untuk peratusan berat yang tinggi. Halaju dan tekanan mempunyai tren yang sama tetapi distribusi mereka tidak rata dalam soldier. Halaju dan tekanan berkurangan dengan pertambahan peratusan berat perak. Distribusi perak dipersembahkan dan dikesahkan melalui experiment. Data daripada experimen dan simulasi mempunyai persamaan yang menyakinkan. Perak didapati berkumpul di kawasan atas soldier. Trajektori partikel juga dikaji untuk menentukan lompang yang mungkin berlaku dalam PDMS soldier. Didapati bahawa banyak trajektori jika peratusan berat perak bertambah dan implikasi ini akan menambah kebarangkalian berlakunya lompang dalam soldier.

ABSTRACT

Electronic packaging plays a very crucial role in an electronic industry. Evolution of electric components happens from non-stretchable to stretchable electronics. PDMS is commonly used in producing stretchable electronics. However, solder made from PDMS has weaker electric conductivity while stretched. This happens to be the interconnectivity among the filler material (Silver) inside the solder is not established well. Due to previous failure in interconnectivity among silver powder, silver flakes are simulated to study the distribution inside the solder. The filler material is treated as particles to run simulation for interaction between VOF and DPM. Different weight percentages of silver filler are selected for simulation. The weight percentages seems to have effect on the distribution, wetting time, velocity and pressure. The wetting time tends to prolong with higher silver percentages. Velocity and pressure distribution shows similar trend for different weight percentages of silver fillers but they are not evenly distributed within the solder. The velocity and pressure decreases as the weight percentage of the silver increases. The distribution of the silver flakes are shown and verified with an experiment and the silver particles tend to accumulate at the upper region of the solder. The experimental and simulation model shows a good agreement. The silver filler tends to accumulate at the top of the solder regardless the silver weight percentages. The trajectories of the particles are also studied to determine possible voids formation in the PDMS solder. There are more trajectories as the silver weight percentage increases which in turn will increase the probability of void formation within the solder material.

LIST OF ABBREVIATION

Ag	Argentum/ Silver
DPM	Discrete Phase Modelling
FVM	Finite Volume Method
IMC	Intermetallic contact
PCB	Printed Circuit Board
PDMS	Polydimethylsiloxane
PSC	Polymer Solar Cell
SCI	Stretchable Conductive Ink
SEM	Scanning Electron Microscope
TIM	Thermal Interface Material
VOF	Volume of Fluid

TABLE OF CONTENT

LIST OF TABLE

LIST OF TABLES

LIST OF GRAPHS

CHAPTER 1

INTRODUCTION

1.0 Background

Electronic packaging is a major discipline within the field of electronic engineering, and includes a wide variety of technologies. Nowadays, there are a lot of electronic products available in the market. As time pass, we can observe the revolution of electronics in our modern days. In the ever-changing technology landscape, the industry has responded and will continue to respond to competitive demand in the global marketplace. It can be observed that the advancement of the technology have pushed the beyond imagination where we can use smartphones, get aid from robots to replace labor force and enjoy using household electrical appliances.

All these electronics appliances consist or made from printed circuit board (PCB). PCBs are boards that mechanically supports and electrically connects electronic components with conductive tracks, pads and other features etched from copper sheets laminated onto non-conductive substrate. Components like capacitors, resistors or active devices are generally soldered on the PCB. PCB is the main component used in an electronic packaging process. Electronic packaging is revolutionizing from using a solid, brittle PCB to a stretchable PCB. A stretchable PCB has been designed for applications that are able to deform according to human body, devices that are made in one size and are accommodated to their final shape, to improve the reliability of devices subject to strains.

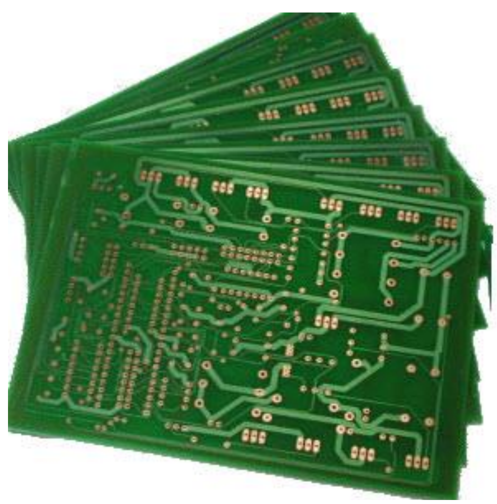

Figure 1-1 A conventional PCB

One of the materials used in manufacturing stretchable PCBs is polydimethylsiloxane (PDMS). Polymers are used in making into PCBs where conventional PCB used metals as they have good electrical conductivity. However, through inventions and innovation, PCBs are now able to be made from stretchable polymer which is an electrical insulator. This is a leap in technology where PCBs can be made from cheaper material (polymer) despite posing stretching and bending properties.

Figure 1-2 Picture of a stretchable PCB

In the manufacturing solutions nowadays, soldering of a stretchable PCB is used with conductive metal ink – Sn-Ag-Cu (SAC). The material consist of tine, silver and copper. The solder is a fusible metal alloy used to create a permanent bond between metal workpieces. Due to the non-elastic properties of SAC, stretching seems impossible for the solder. To permit best performance of the stretchable PCB, the solder should also follow the stretching of PCB.

From the implications of stretchable PCB, stretchable conductive ink (SCI) is introduced in the electronics manufacturing. The SCI which is introduced in to the manufacturing process is PDMS-silver solder. PDMS provides the elasticity to the solder while silver acts as the filler material to conduct electricity within the solder. In addition, PDMS is transparent at optical frequencies from 240 nM to 1100 nM. This helps in the observation in micro-channels visually using a microscope. PDMS is more likely to be applied in medical industries as they are considered as bio-compatible. PDMS have shown good properties in making wearable or stretchable PCB.

As mentioned earlier, SAC has always been used in the soldering process of stretchable PCB. However, the advent of PDMS – Ag materials make a new possibility to replace SAC in the solder joint. PDMS – Ag is low cost and has good electrical conductivity. It will be a big advantage to electronic industries as PDMS – Ag may be effective in reducing capital required in manufacturing due to its low cost.

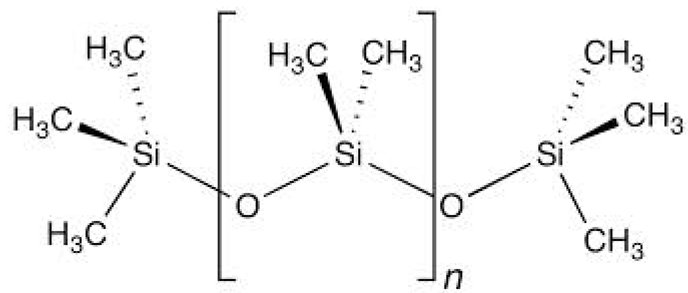

Figure 1-3 Chemical formula of PDMS

The capabilities of the PDMS have shown the possibilities of revolutionizing the electronics industries.

1.1 Problem Statement

PDMS-Ag or stretchable conductive ink is a new material in soldering material in stretchable circuit board. The reflow of the solder has to be study and conform to the IPC standard. Intermittent electrical properties occur while using PDMS with silver particles (spherical) while stretched. To overcome this problem, silver flakes are proposed in the material. Hence, the reflow and particle tracking of the PDMS with silver flakes are to be observed with computational tool – ANSYS fluent.

1.2 Objectives

There are several objectives are set to be achieved in this project:

1. To simulate the reflow process of SCI on PCB and validate with experiment.
2. To study and verify the distribution of silver flakes in a solder joint.
3. To determine the fillet height and angles of the solder joint.

1.3 Scope and limitations of the study

Simulation is the main scope in this study. The reflow process of SCI and the distribution of the filler materials (silver flakes) are to be simulated in this study. Silver flakes used are not spherical and they are have irregular shapes. The reflowing time are simulated with volume of fluid and the distribution of the silver flakes are simulated with discrete phase modeling (DPM). Both reflow and distribution are simulated using ANSYS FLUENT. The distribution of the silver flakes is simulated by treating them as particles and track them.

Validation with experimental data obtained from SCI Jabil will be conducted with the simulation data. The experiment to observe the distribution of the silver flakes is done in Jabil. SEM investigation is done for observing the microstructural. Captured images from the experiment will be compared with the simulation data. The limitation of the current experimental setup however, is that the experiment needs to be conducted only in Jabil with limited specimen prepared for the validation due to cost restriction.

1.4 Overview of the study

This project entails simulation on the reflow of the new material solder which is made of polydimethylsiloxane and silver flakes. There is various simulation done on the reflow process of the solder. There are several models used in modelling the wetting angle of the solder. The methods of modelling are reviewed and a new model is constructed with ANSYS FLUENT.

The PDMS-Ag solder is modeled to adhere to the wall of the capacitor. The solder will flow and producing a fillet or chamfer attaching to the walls of capacitor. The fillet angles are to be determined. The simulation of the fillet has to be conform to the IPC standard as provided by Jabil.

Particles tracking are an important factors in determining the propagation of silver flakes in the PDMS using DPM models. The silver flakes are described as particles to be injected and observe the flow within the solder. It is the factor in determining the silver filler distribution. Drag law are introduced given the the non-spherical shape of the silver flakes. The particles tracking is used to observe the distribution of the silver flakes inside the PDMS solder to give a clear picture on the silver filler interconnection that subsequently will lead to better electrical conductivity.

CHAPTER 2

LITERATURE REVIEW

2.0 Introduction

The solder reflow of stretchable conductive ink is a process in electronic packaging. Researches on the electronic packaging and simulation on the packaging is done. In the reflow process, soldering is done on stretchable PCB. The newly developed stretchable conductive ink made from PDMS-silver requires study from predecessor like SAC solder for the simulation. Lastly, the usage of DPM simulation in specific areas is studied too so that DPM can be used in vast application.

2.1 Electronic Packaging

Electronic packaging is a process that requires assemblies of electronic component into a PCB and lastly into a product. There are some studies related to the electronic packaging where vast studies are done like SMT technologies, soldering process investigation and others. In electronics packaging, thermal analysis is very important. High temperature difference in solder reflowing process is not good as it may cause defects in the PCB. Simulations are done on the thermal stress where it is found out that solder ball root will form the nucleation of initial crack and degrade the thermal cycle life time. The stress will alleviative in the solder joint when the baking is performed after the solder reflow process.[3] The strength of the electronics are greatly affected during electronic packaging process. Nano-electronic packaging with the usage of a novel nanocomposite TIM helps in heat dissipation process. Heat is also a concern in electronic packaging where it can reduce the lifetime of the electronics. In Figure 2-1, the TIM has higher thermal stress where heat dissipation is better than before. Experimentation on heat dissipation is also always an issue in electronics industry. [2]

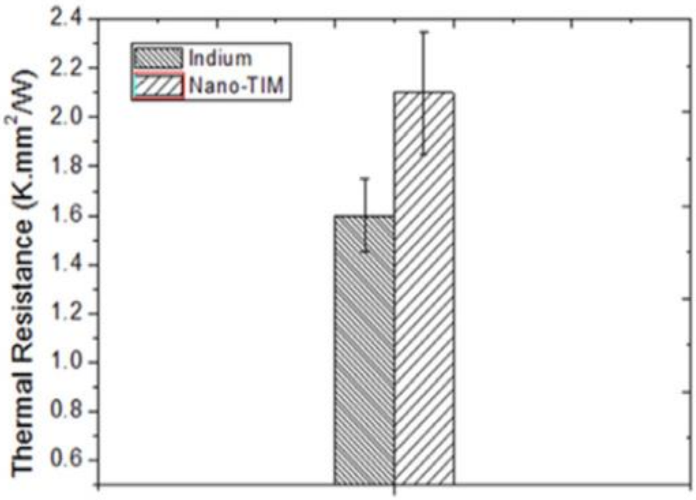

Figure 2-1 Thermal stresses of TIM[2]

For soldering process, the solidification of the solder is also important. A study done on SAC solder solidification are most found using ANSYS simulation. The formation of solidification defects in lead-free soldering is greatly influenced by material factors as well as the design of circuit assemblies. The stress distribution of the assembly during reflow to influence the formation of solidification defects.[4]

IMC region has always been the central topic in electronic packaging. Investigation on the fully developed Cu_3Sn in electronic packaging is done to determine the shape and voids within the solder. Soldering pressure higher than 1 N can be also used to obtain a full Cu3Sn solder joint. But increasing the soldering pressure is not only unnecessary but also

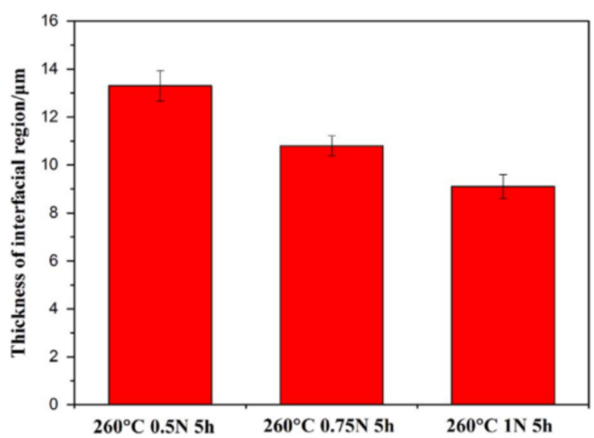

Figure 2-2 Thickness of IMC according to solder stress

risky, because it may cause excessive Sn overflow, which can lead to short-circuits in finepitch interconnection. [5] Comparison of different solders on formation of intermetallic layer. The solder used is SAC305/Ag/Cu and SAC0705-3.5Bi-0.05Ni/Ag/Cu. The voids appear inside the (Cu, Ni)$_6$Sn$_5$ layer instead of at the interface between the IMCs and the substrate. It is suggested that the voids are formed due to the gap between IMC grains during the formation and growth of IMCs. The probability to form large plate-like Ag_3Sn is higher in SAC305/Ag/Cu than in SAC0705-Bi-Ni/Ag/Cu due to a higher Ag concentration. The large Ag3Sn located at both the soldering interface and the bulk solder depends on the distribution of Ag element. As opposed to Cu_6Sn_5, (Cu, Ni)$_6$Sn$_5$ can effectively suppress the formation and growth of Cu_3Sn. Therefore, the formation of Kirkendall voids can be limited by adding a small amount of Ni to SAC solder alloys.[6]

Voids in electronic packaging will affect the strength of the solder. The effect of void percentage in the solder layer on the shear strength and thermal property of DA3547 packages by SAC soldering technology is studied in a paper. Additionally, voids in the solder layer may cause stress concentration. With more voids inside, the solder layer shows a higher stress concentration. These stress concentration positions are suggested to be the initial parts for crack under ambient loads.[7] Modelling of the KIRKENDALL voids are done to determine the effect. Numerical simulations on the material point level provide insight into the mechanisms of failure by formation and growth of KIRKENDALL voids and show the potential of the model for the failure analysis of joints.[8]

The wetting of the solder are determined by the contact angle. The study of wetting behaviour is an important step in the characterisation of solder alloys and requires the discussion of different parameters that affect the solder junctions. Increasing the surface tension value does not have a high influence on the solder shape. The melted solder is greatly influenced by the contact angle and, to a smaller extent, by the surface tension, which controls the height of the melted sample.[9] The importance of contact angle in soldering is highlighted here.

FEM is done on the solder reflowing process in a more complex way where FSI is involved. A methodology of thermal coupling method for board-level BGA assembly for an infrared-convection oven. In the present study, a thermal coupling method using the code coupling software MpCCI was utilized.[3]

Heat transfer in solder reflow process is also an important factor in solder reflowing. Simulation on the heat transfer is done with computational tool. he moderate inclination of PCB decreases the thickness differences of the condensate layer, thus it considerably improves heat transfer uniformity. It also decreases the temperature differences of the PCB, which is an ultimate goal of a proper and optimised reflow soldering process setup. [10]

2.2 Stretchable electronics

Due to advancement in technology, bendable or stretchable electronics are widely used especially in medical industries. Stretchable or bendable electronics are mostly applied in wearable devices. Fabrication of bendable PCB using PDMS. Tests are done. Procured PDMS liquid substrate could be used to control the depositing morphologies of coalesced Ag precursor inkjet droplets. Then, semi-wrapped lines were fabricated on the PDMS surface. After the printed deposits were reduced to AgNPs by the in situ vapor phase reduction, a conductive film with good transparency and high bendability was fabricated. [11] The stretch ability of the PDMS circuit has been amazing and gives possibilities of developing new products. A method of producing stretchable electronics that is simple and cost effective is also introduced. Fabrication of Ag-PDMS composites is simple and cost effective in [12]. This shows the possibly of high return for stretchable circuit.

The conductivity of the Ag-PDMS stretchable nanocomposites is also an important issues in electronic industry. Methods of improving the electrical response of Ag-PDMS is proposed in [13] where surfactant-free Ag NPs that were fabricated in situ by laser ablation of a silver target into a PDMS prepolymer and toluene solution are able to show improvement in electrical response. This show PDMS is able to be applied in electronics industry. The rough PDMS substrates were found to significantly assist the spin coating of solution based Ag nanoparticles films and their adhesion owing to the viscous frictional effects of the roughness pattern. The presence of random micro ridges on PDMS can be considered as a useful application of roughness enhanced stretch ability of metal-polymer.[14]

Application of PDMS are used in various applications. Electrodes also shows elastic properties. The electrodes are made up of Ag-PDMS. In [15], the paper measures the electrical properties of a single cell and determines the conductivity of the material according to the silver concentration. Stretchable polymer solar cells (PSE) are also new applications in stretchable electronics. Their mechanical stability and power conversion efficiency (PCE) thus are still far below the requirement for the practical applications. Improvement on the mechanical robustness of PSE is also done and the study on the efficiency after stretched is also done. [16]

PDMS is also applied in electronic skin application. Stretchable sensors have also been made by fabricating a temperature sensor onto an elastomeric substrate. Another class of organic electronic devices that has also been made stretchable is organic light-emitting diodes (OLEDs).[17] There are vast applications in stretchable electronics. However, the stretchable conductive ink or solder is not shown in papers for reference. The study on PDMS solder is new for the electronics industry.

2.3 Discrete Phase Modelling

DPM is capable of tracking particles inside fluid flow. For studies nowadays, DPM are always applied in areas like combustion, visualization, chemical reactions, drying and particle formation process. The coal combustion in a pusher type reheating furnace is modelled with DPM. DPM is used to model the transport of coal particles. The tracks of the coal particles are illustrated in Figure 2-3. [1]

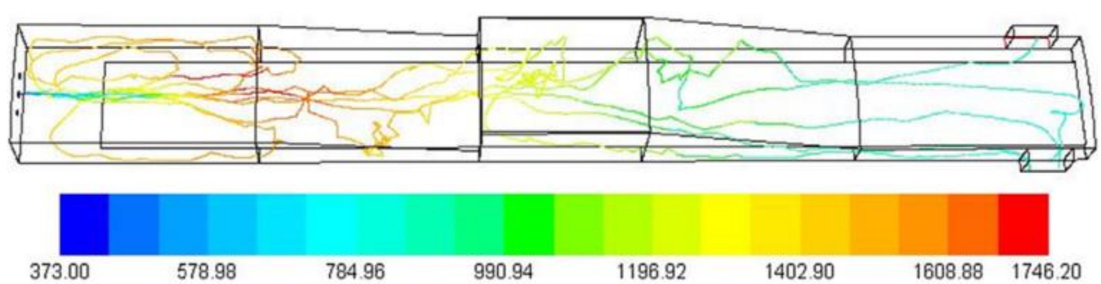

Figure 2-3 Tracks of coal combustion particles[1]

DPM also shows its versatility by simulating the sticking process of S. aureus bacterium. The bacterium are treated as particles in DPM. The presented models are universal can be adapted for different kinds of bacteria as well as their interaction with different surfaces. The modelling of the contact and sticking process was represented by applying two kinds of models, a simpler adhesive viscous elastic and a more realistic adhesive viscous elastic-plastic interaction model.[18]

DPM is also applied in simulation of fiber reinforced concrete. The fracture of the concrete is simulated and the ruptured fibre are considered as particles in simulation. The model has shown as an accurate and efficient simulation tool for studying the mechanics of the evolution of fracture processes of fiber reinforced concrete.[19]

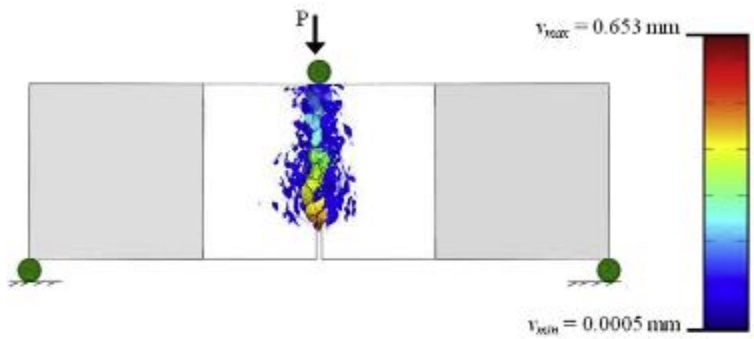

Figure 2-4 Study of fracture of concrete using DPM

Another simulation using DPM is done on gas particle flow. A three-dimensional simulation was performed on the turbulent gas–solid flow in a cylindrical channel with opposed round jets. The gas-particle flow behaviours, especially the vortex structure evolution, particle motion, time-averaged velocity profiles and turbulence intensity were able to be investigated using DPM.[20]

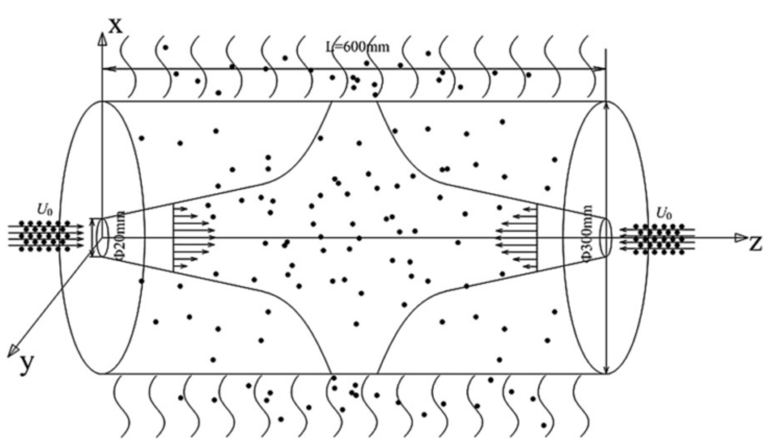

Figure 2-5 Sketch of the geometry of round jets model

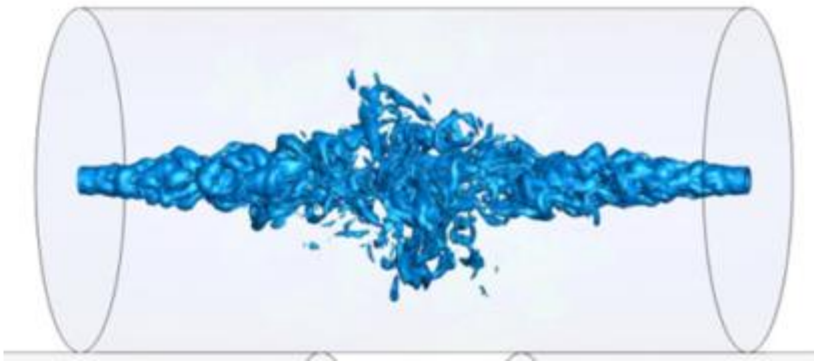

Figure 2-6 Simulation results of the gas jets model

A numerical study is carried out to assess the influence of bubble injection characteristics on the mixing behaviour in a 2-D gas-solid fluidized bed at high pressures. DPM is applied to separate the particles from the gas bubbles; hence, the interaction between the particles and gas bubbles can be studied.[21]

From the study of DPM, vast application can be applied like approximation of bacterium as particles. Hence, DPM for the silver flakes in solder can be applied as this is new research in the electronic packaging. From the researches so far, there is no DPM application in electronic packaging. Hence, DPM will be done in this research.

CHAPTER 3

METHODOLOGY

3.0 Introduction

ANSYS workbench will be utilized to simulate the solder reflowing process of PDMS-silver solder. Fluent in ANSYS is chosen as the simulation tool. The simulation conducted will observe the wetting/reflowing of the solder and also silver distribution inside the solder. There are several settings/models and theories involved for the ANSYS simulation. The models involved are:

- Laminar model
- Discrete Phase Model (DPM)

There are also concerns needed for the simulation:

- Properties of PDMS
- Properties of silver
- Shape factor
- Wetting angle/ contact angle of PDMS to PCB substrate
- Concentration of the silver flakes

Under the DPM, there are a few theories available behind it:

- Pressure gradient force
- Saffman lift force
- Thermophoretic force
- Virtual mass force

The modeling process requires these theories to back up the simulation.

3.1 Preparation for the modeling of solder reflowing

Before starting the ANSYS simulation on the solder reflowing, some data are collected to proceed with the process. These data are crucial to ensure the appropriateness of the simulation. The data will be required in the computation of the reflowing process.

The outline of the model is defined beforehand. The reflowing process is done on PCB substrate to solder the capacitor. The scale of the model has to be determined beforehand. The simulation is done on millimeter scale which is on a capacitor in PCB. Only one capacitor is simulated for the reflowing results. It is because the model will be redundant if simulating the whole PCB reflowing process. The reflowing processes within the PCB is similar for each component. Hence, a part in the PCB is selected and cropped out for simulation. The dimension of the capacitor is as below:

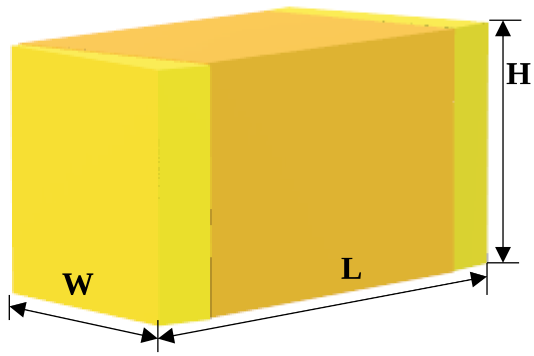

Figure 3-1 Figure of a capacitor

Table 1 Dimension of a capacitor

L (mm)	0.4
W (mm)	0.2
H (mm)	0.2

Besides that, the solder material has to be determined. The solder used is stretchable conductive ink which is composed of PDMS with silver filler. PDMS is a polymer which is unable to conduct electricity; thus, the filler material – silver will be added for electricity conduction. Previously, the filler used is spherical shape. Now, the model will be using silver flakes as the filler. The properties of the PDMS is shown below:

Table 2 Properties of PDMS

Density (kg/m^3)	**965**
C_p specific heat (J/kg K)	1.72
Thermal conductivity (W/mK)	0.001
Viscosity (kg/ms)	0.65
Molecular weight (kg/kmol)	162
Standard state enthalpy (J/kg mol)	0.04
Solidus/liquidus temperature (°C)	100
Surface Tension (N/m)	15.9

The filler material – silver is approximated as particles to be used in DPM. Hence, there are some properties needed to be determined, for example: density, particle diameter, specific heat and etc. The properties are tabulated in Table 3:

Table 3 Properties of silver filler

Density (kg/m^3)	**10500**
Particle diameter (approx) (mm)	0.001
Specific heat constant (J/kg K)	238.65
Thermal conductivity (W/m K)	406

3.2 Mathematical model and governing equations

3.2.1 Volume of fluid

3D simulation of a 01005 capacitor with PDMS – silver solder will be conducted. The simulation will be modeled with Eulerian continuous phase flow and the newly implemented DPM model. For the continuous flow, the concern is on the wetting of the molten solder (PDMS – silver). Therefore, Navier Stokes equation will be utilized in this simulation to govern mass transfer of the fluid. Navier Stokes equations consist of continuity, momentum and energy:

Continuity equation

$$\frac{\delta\rho}{\delta t} + \nabla \cdot (\rho\boldsymbol{u}) = 0 \quad \textbf{(1)}$$

$$\frac{\delta\rho}{\delta t} + \frac{\delta(\rho u)}{\delta x} + \frac{\delta(\rho v)}{\delta y} + \frac{\delta(\rho w)}{\delta z} = 0 \quad \textbf{(2)}$$

Momentum equation

X-momentum:

$$\frac{\delta(\rho u)}{\delta t} + \frac{\delta\left(\rho u^2\right)}{\delta x} + \frac{\delta(\rho uv)}{\delta y} + \frac{\delta(\rho uw)}{\delta z} = -\frac{\delta p}{\delta x} + \frac{1}{Re_r}\left(\frac{\delta\tau_{xx}}{\delta x} + \frac{\delta\tau_{xy}}{\delta y} + \frac{\delta\tau_{xz}}{\delta z}\right) \quad \textbf{(3)}$$

Y-momentum:

$$\frac{\delta(\rho v)}{\delta t}+\frac{\delta(\rho uv)}{\delta x}+\frac{\delta(\rho v^2)}{\delta y}+\frac{\delta(\rho vw)}{\delta z}=-\frac{\delta\rho}{\delta y}+\frac{1}{Re_r}\left(\frac{\delta\tau_{xy}}{\delta x}+\frac{\delta\tau_{yy}}{\delta y}+\frac{\delta\tau_{yz}}{\delta z}\right) \quad \textbf{(4)}$$

Z-momentum:

$$\frac{\delta(\rho w)}{\delta t}+\frac{\delta(\rho uw)}{\delta x}+\frac{\delta(\rho vw)}{\delta y}+\frac{\delta(\rho w^2)}{\delta z}=-\frac{\delta\rho}{dz}+\frac{1}{Re_r}\left(\frac{\delta\tau_{xz}}{\delta x}+\frac{\delta\tau_{yz}}{\delta y}+\frac{\delta\tau_{zz}}{\delta z}\right) \quad \textbf{(5)}$$

Energy equation:

$$\frac{\delta E_T}{\delta t}+\frac{\delta(uE_T)}{\delta x}+\frac{\delta(vE_T)}{\delta y}+\frac{\delta(wE_T)}{\delta z}=-\frac{\delta(u\rho)}{\delta x}-\frac{\delta(v\rho)}{\delta y}-\frac{\delta(w\rho)}{\delta z}-\frac{1}{Re_rPr_r}\left(\frac{\delta q_x}{\delta x}+\frac{\delta q_y}{\delta y}+\frac{\delta q_z}{\delta z}\right)+$$
$$\frac{1}{Re_r}\left(\frac{\delta}{\delta x}\left(u\tau_{xx}+v\tau_{xy}+w\tau_{xz}\right)+\delta\left(u\tau_{xy}+v\tau_{yy}+w\tau_{yz}\right)+\frac{\delta}{\delta z}\left(y\tau_{xz}+v\tau_{yz}+w\tau_{zz}\right)\right) \textbf{(6)}$$

Where

$\rho = density\ of\ fluid$

$u = velocity\ in\ x - direction$

$v = velocity\ in\ y - direction$

$w = velocity\ in\ x - direction$

$\tau = shear\ stress$

$E_T = Total\ energy$

$Re_r = Reynold\ Number$

$\mathrm{Pr_r} = Prandtl\ Number$

There are multiphase involved in the solder reflowing model where two phases (air and PDMS solder) are not interpenetrating. Hence, the interaction between these two fluids can be modeled with volume of fluid (VOF).

In this model, the interaction of the PDMS solder with the air are associated with the surface tension coefficient. The surface tension between these two phases are responsible for the wetting process of solder on PCB. The surface tension of PDMS is 15.9 N/m. It allows the solder interacts with air and wets the PCB to form a fillet fixing the electronic components to the PCB. The model of the reflowing of the solder can be illustrated as in Figure 3-2:

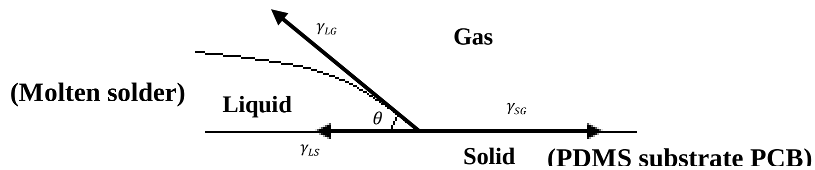

Figure 3-2 Figure of the model of solder with surface tension

According to Young's equation, when a liquid comes into contact with a solid in a bulk, gaseous phase, there is a relationship between the contact angle, θ and the surface tension of the liquid, γ_{LG}, the interfacial tension, γ_{SL} between liquid and solid, and the surface free energy, γ_{SG} of the solid. For the simulation of the solder reflowing, the contact angle need to be determined to portray the adhesion. The contact/wetting angle of the molten solder is very important to ensure the pattern of the solder is similar to the solder reflowing process. The Young's equation is equated as below:

$$\gamma_{SG} = \gamma_{LS} + \gamma_{LG} \cos \theta \qquad \textbf{(7)}$$

Where

$\gamma_{SG} = surface\ tension\ of\ the\ solid - gas\ boundary$

$\gamma_{LG} = surface\ tension\ of\ the\ liquid - gas\ boundary$

$\gamma_{LS} = surface\ tension\ of\ the\ liquid - solid\ boundary$

$\theta =$ Contact/wetting angle

In this case, the wetting of the molten solder is modeled in a simplified model where surface roughness is not considered.

Besides that, volume of fluid (VOF) will be adapted in the simulation. VOF is a free surface modeling technique. It is a numerical technique to track and locate free surface. VOF is also an Eulerian method which is characterized by a mesh that is either stationary or is moving in a certain prescribed manner to accommodate the evolving shape of the interface.

VOF formulation relies on the fact that two or more fluids are not interpenetrating. In this case, the molten solder (liquid) interacts with the air (gas) where both phases do not diffuse to each other. The air is defined as the primary phase while the molten solder is defined as the secondary phase. VOF is an advection scheme. Hence, it is a numerical recipe where we can track the shape and position of the interface. In addition, VOF and Navier-Stokes equation have to be solved separately in this model. VOF tends to track the shape and position while Navier-Stokes computes the flow phase of the molten solder.

The tracking of the interface between the molten solder and air is accomplished by the solution of continuity equation for volume fraction of one of the phase. The equation of the VOF can be represented as below:

$$\frac{1}{\rho_q}\left[\frac{\delta}{\delta t}\left(\alpha_q \rho_q\right) + \nabla \cdot \left(\alpha_q \rho_q \vec{v}_q\right)\right] = S_{\alpha_q} + \sum_{p=1}^{n}(\dot{m}_{pq} - \dot{m}_{qp}) \quad \textbf{(8)}$$

Where

$\dot{m}_{pq} = mass\ transfer\ from\ air\ (phase\ p)\ to\ molten\ solder\ (phase\ q)$

$\dot{m}_{qp} = mass\ transfer\ from\ molten\ solder\ (phase\ q) to\ air\ (phase\ p)$

In this case the mass transfer from p to q and vice versa are considered the same. The source term, S_{α_p}, is zero as there is no addition of the other phase into the model. In addition, the VOF/ volume fraction equation will not be solved for the primary phase (air). The primary-phase volume fraction will be computed based on the following constraint:

$$\sum_{q=1}^{n} \alpha_q = 1 \quad \textbf{(9)}$$

The VOF/volume fraction equation can be solved using implicit or explicit time discretization. In this model, implicit model is chosen. Implicit methods require extra computation and is harder to implement. However, it is more stable over a wide range of time and constitute excellent iterative solvers for steady-state problems.

For the implicit solver, the discretization of the volume fraction equation can be represented as below:

$$\frac{\alpha_q^{n+1}\rho_q^{n+1}-\alpha_q^n\rho_q^n}{\Delta t}V+\sum_f\left(\rho_q^{n+1}U_f^{n+1}\alpha_{q,f}^{n+1}\right)=0 \qquad \textbf{(10)}$$

Where

$n+1 = index\ for\ new\ (next)\ time\ step$

$n = index\ for\ previous\ (current)\ time\ step$

$\alpha_{q,f} = face\ value\ of\ the\ q^{th}\ volume\ fraction$

$V = volume\ of\ cell$

$U_f = volume\ flux\ through\ the\ face, based\ on\ normal\ velocity$

Since this equation requires the volume fraction values at the current time step (rather than at the previous step, as for the explicit scheme), a standard scalar transport equation is solved iteratively for each of the secondary-phase volume fractions at each time step.

3.2.2 Dispersed Phase Method (DPM)

In addition to solving the transport equation of the continuous flow of the molten solder, DPM allows us to simulate discrete second phase in a Lagrangian frame of reference. Commonly, the second phase is modeled as spherical particles dispersed in the continuous phase. With this, FLUENT computes the trajectories of these discrete phase entities, as well as heat and mass transfer to or from them.

In this model, the silver flakes is injected into the molten solder as particles. ANSYS FLUENT is able to do calculation of discrete phase trajectory using a Lagrangian formulation that includes discrete phase inertia, hydrodynamic drag and the force of gravity for both steady and unsteady flow.

Trajectory Calculation

The calculation of the trajectory of the silver flakes within the molten solder is important as it determines the interaction between the silver flakes and molten solder. Hence, there are a few equations of motion for particles governing the model is needed.

3.2.2.1 Particle Force Balance

DPM is used to simulate the flow of the silver flakes. Using FLUENT, the trajectory of the silver flakes can be determined. The particles have to be dispersed in the molten solder through injection. Hence, a two-way interaction between the dispersed phases (silver flakes) and the continuous phase (molten solder) is simulated. The continuous phase is solved based on Eulerian model. On the other hand, the discrete/dispersed phase is a Lagrangian reference frame. FLUENT can predict the trajectory of the discrete phase particle by integrating the force balance on the particles. The forces experience by the particle can be shown in Figure 3-3.

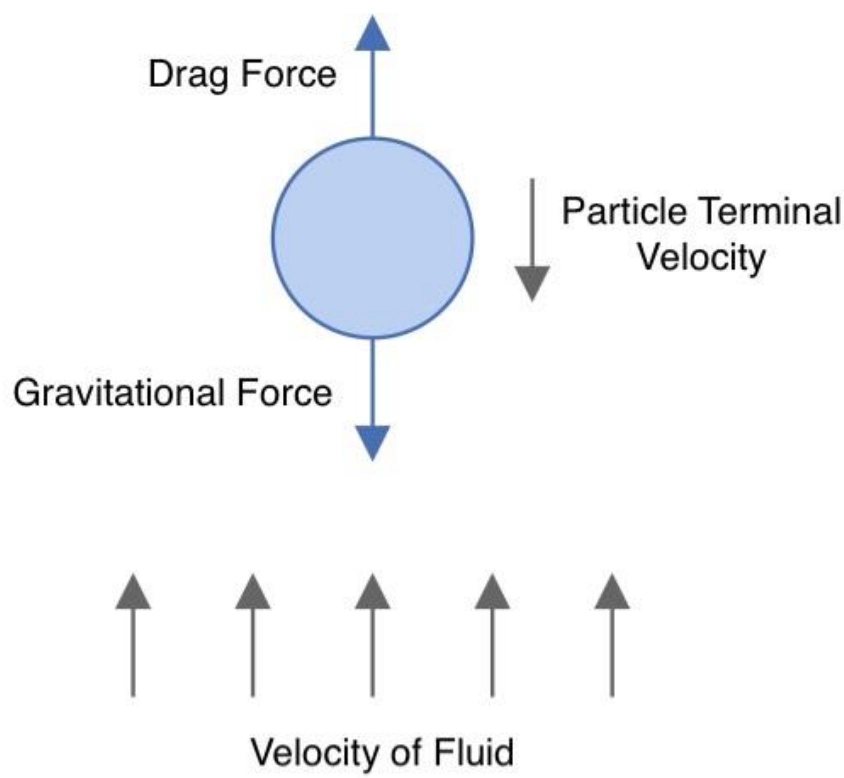

Figure 3-3 Forces experience by a particle

The force balance equates the particle inertia with forces acting on the particle and can be written as:

$$\frac{du_p}{dt} = F_D\left(u - u_p\right) + \frac{g_x\left(\rho_p - \rho\right)}{\rho_p} + F_x \quad \textbf{(11)}$$

Where:

$F_D(u - u_p) = drag\ force\ per\ unit\ particle\ mass$

$u = fluid\ phase\ velocity$

$u_p = particle\ velocity$

$\rho = fluid\ density$

$\rho_p = particle\ density$

The drag force can be represented as below:

$$F_D = \frac{18\mu}{\rho_p d_p^2}\frac{C_D Re}{24} \quad \textbf{(12)}$$

The Reynolds number, Re is defined as

$$Re = \frac{\rho d_p\left|u - u_p\right|}{\mu} \quad \textbf{(13)}$$

In this simulation model, the silver flakes is defined as non-spherical particles. The drag coefficient will be modified as the formula below:

$$C_D = \frac{24}{Re}\left(1 + b_1 Re^{b_2}\right) + \frac{b_3 Re}{b_4 + Re} \quad \textbf{(14)}$$

Where

$b_1 = \exp(2.3288 - 6.4581\phi + 2.4486\phi^2)$

$b_2 = 0.0964 + 0.5565\phi$

$b_3 = \exp(4.905 - 13.8944\phi + 18.4222\phi^2 - 10.2599\phi^3)$

$b_4 = \exp(1.4681 + 12.2584\phi - 20.7322\phi^2 + 15.8855\phi^3)$

The drag coefficient has a crucial role in solving the particle tracking of DPM. However, for non-spherical particles, the drag coefficient has to be modified as shown in equation (14). The symbol ϕ represents shape factor which is the approximation of the sphere shape. It is the measure of how closely the shape of an object approaches that of a mathematically perfect sphere.

$$\phi = \frac{A_s}{A_p} \tag{15}$$

Where A_s is the surface area of a sphere having the same volume as the particle and A_p is the actual surface area of the particle.

Shape Factor

The formulation of the shape factor can be represented as below:

The surface area of sphere is A_s and the volume of particle is V_p. The formula requires to write the surface area of the sphere in terms of particle:

$$A_s^3 = (4\pi r^2)^3 = 4\pi(4^2\pi^2 r^6) = 4\pi \cdot 3^2\left(\frac{4^2\pi^2}{3^2}r^6\right) = 36\pi\left(\frac{4\pi}{3}r^3\right)^2$$

$$A_s^3 = 36\pi V_p^2$$

$$A_s = \left(36\pi V_p^2\right)^{\frac{1}{3}} = 6^{\frac{2}{3}}\pi^{\frac{1}{3}}V_p^{\frac{2}{3}} = \pi^{\frac{1}{3}}\left(6V_p\right)^{\frac{2}{3}}$$

Hence,

$$\phi = \frac{A_s}{A_p} = \frac{\pi^{\frac{1}{3}}\left(6V_p\right)^{\frac{2}{3}}}{A_p} \tag{16}$$

With this derivation, the shape factor of the silver flakes can be determined with the surface area and volume of the particle. Furthermore, the silver flakes in this model are portrayed as an <u>ideal cylinder</u>. Therefore, the shape factor of the silver flakes can be calculated as:

$$h = 2r$$

$$A_p = 2\pi r(r+h) = 6\pi r^2$$

$V_p = \pi r^2 h = 2\pi r^3$

$$\phi = \frac{\pi^{\frac{1}{3}}(6 \cdot 2\pi r^3)^{\frac{2}{3}}}{6\pi r} \approx 0.874$$

The shape factor of the silver flakes will be 0.874.

3.2.2.2 Thermophoretic force

Thermophoretic force is a resultant from thermophoresis process. Thermophoresis is a phenomenon observed in mixtures of mobile particles where the different particle types exhibit different responses to the force of a temperature gradient. The thermophoretic force depends on the temperature gradient in the surrounding gas molecules.

The formula of the themophoretic force is:

$$F_x = -D_{T,p} \frac{1}{m_p T} \frac{\delta T}{\delta x} \tag{17}$$

Where

$D_{T,p} = Thermophoretic\ coefficient$

The interaction of particles with thermophoretic force can be represented in Figure 3-4.

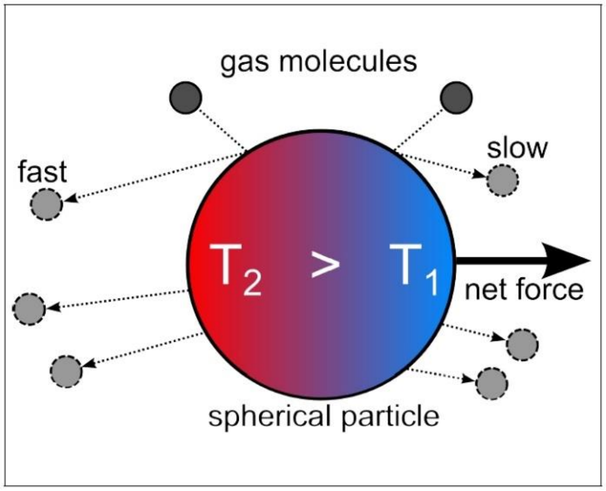

Figure 3-4 Interaction of particle with thermophoretic force

3.2.2.3 Brownian Motion

The motion of the particles can be described as Brownian motion. Brownian motion is the random motion of particles suspended in a fluid resulting from their collision with the fast-moving atoms or molecules in the gas or liquid. The motion described by the Brownian motion can be described as in Figure 3-5.

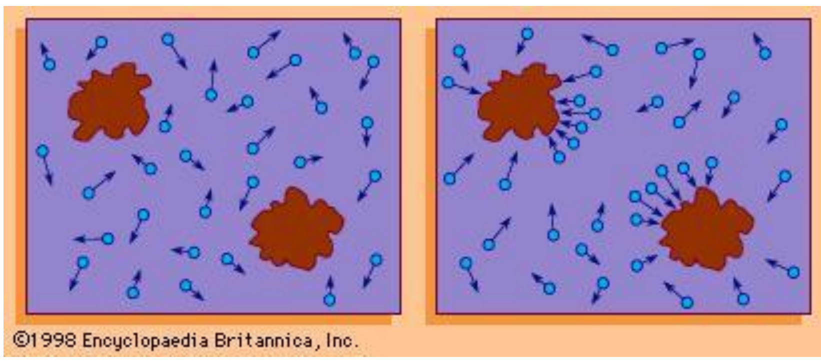

Figure 3-5 Random motion of a Brownian particle

In the ANSYS simulation, the components of the Brownian force are modeled as a Gaussian white noise process intensity $S_{n,ij} = S_0\delta_{ij}$

Where δ_{ij} is the Kronecker delta function, and

$$S_0 = \frac{216\nu\sigma T}{\pi^2 \rho d_p^5 \left(\frac{\rho p}{\rho}\right)^2 C_c} \quad \textbf{(18)}$$

Where

$T = Absolute\ temperature\ of\ the\ fluid$

$\nu = Kinematic\ viscosity$

$\sigma = Stefan - Boltzmann\ constant$