Molecular dynamics simulation of the nano-reinforced lead-free solder at different reflow soldering process temperature

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Abstract. Temperature plays an important role in the reflow soldering process. Reflow soldering process which involves four basic stages including preheating, soaking, reflow and cooling require a specific range of temperature at each stage and the highest temperature is the reflow stage. In this study, the movement of the reinforced nanoparticles in the lead-free solder at three different stage temperatures which are 30°C, 150°C and 250°C will be shown via Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software. The simulation model able to show the movement of nanoparticles in the solder at three different reflow soldering process stages. The most vigorous movement of nanoparticles is shown at the temperature of 250°C while the least vigorous movement is shown at room temperature of solder which is at 30°C.

1 Introduction

Most of today’s electrical and electronic equipment which commercially manufactured are using surface mount technology (SMT) as it gives ample advantages to replace through-hole technology (THT). SMT offers efficient uses of printed circuit board (PCB) space as more electronic components can be packed onto the PCB which next increasing the possibility to build complex electronic circuits. In addition to that, SMT allowing the automated PCB assembly which brings to reduction of manufacturing cost and speed up the manufacturing process which then improving the reliability of electronic assembly.

The reflow soldering is the best method for SMT compared to wave soldering which is more complex as the board temperature and board time spends in the wave soldering machine needs to be carefully monitored. The mistake in maintaining the right wave soldering environment lead to the imperfection in soldering process. Reflow soldering process uses a solder paste out of powdered solder and flux, which then used that paste to attach the electronic components to the contact pads. Next, the entire assembly is being heated in a reflow oven to melt the solder and then connect the joint. Reflow soldering process undergoes four basic stages including preheat, thermal soak, reflow, and cooling.

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In the recent 10 years, the improvement in the solder technology which is the reinforcement of nanoparticles into the solder becomes more vigorously as researchers found out that by adding nanoparticles such as cobalt (1), copper (2), silver (3), nickel (4) diamond (5), ironnickel oxide (6), iron oxide (7), titanium dioxide (8), zinc oxide (9) and many more is proven to increase the solder properties in terms of either one, mechanical, thermal, wetting and intermetallic compound layer or the four of them.

Numerical approaches are introduced in the SMT field to reduce the cost and time-consuming experimental work. This approaches also make ease for showing the reaction of the solder in certain condition clearly and accurately. Over years, there are lots of numerical approaches to simulate the reflow soldering process environment including finite element method (FEM) (10), finite volume method (FVM) (11), fluid-structure interface (FSI) (12), lattice Boltzmann’s method (LBM) (13), discrete phase method (DPM) (14) and molecular dynamic (MD) (15). This paper is focussing on the used of MD to simulate the nano-reinforcement lead-free solder during the reflow soldering process.

2 Methodology

2.1 Simulation tools

The problem is to simulate the solder atom with added nanoparticles in the atomic scale. A molecular dynamics (MD) software and other tools such as the Notepad++, command prompt and Ovito have been used to perform the simulation.

2.1.1 MD software

The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software by Sandia National Laboratories is used to simulate the nano-reinforced solder paste environment. LAMMPS is a free open source software that uses Message Passing Interface (MPI) for parallel communication and it uses neighbor lists (Verlet lists) to keep track nearby particles. LAMMPS has potentials for solid-state material, soft-matter and coarse-grained or mesoscopic systems (16).

2.1.2 Other tools

LAMMPS is executed by reading the commands in the input script (text file) which is written in the Notepad++. To perform the LAMMPS simulation, the input script is read through the command prompt application which is the command line interpreter. Lastly, Ovito is used as the visualization tool to show the trajectory of the nanoparticles in the solder.

2.2 Input script

There are 4 major parts that must be considered in the input script which are initialization, atom definition, settings, and run a simulation. The first one is the initialization part, where the parameters for the simulation is set up. The command such as units, boundary, and atom style is used to express the parameters. The units style for this simulation is set first with any of units style which lj, real, metal, si and others accordingly. The choice of the units style must consider the conversion of parameters unit following the units style. This simulation is set as real. Next, the boundary for the simulation can be set as periodic, fix, shrink-wrapped and shrink-wrapped with a minimum value at x, y and z direction. The
boundary for this simulation is set as periodic in all directions. This shows the atoms can exit at one end and re-enter at the other end. For inter-atomic potential definition, the pair_style command is used to set up the force field style. There are variety of pair_style that can be chose. For this simulation, the lj/cut pair style is used to set the interaction between two different atoms. The command pair_coeff is used to set up the force field coefficient for each interaction of atoms.

Next part is the atom definition. The geometry and the atoms for the simulation model will be created. The commands such as lattice, region, create_box, and create_atoms are commonly used. The dimension of the simulation model can be set up as 2D or 3D and for this simulation it was set as 3D while the lattice is set to face-centered cubic (fcc). Then the region for the simulation model is set up by command region box follows by the required dimension to make a box shape model. To set up two different atoms in a simulation model, command create_box is used to differentiate another atom that is in the region box. The create_atoms command is used to create the solder atoms in the region box. The nanoparticles will be introduced in a sphere region. After the region for the nanoparticles has existed, command delete_atoms is used to delete the atoms in the sphere region so that the new atoms will be created in the sphere by command create_atoms.

The third part is the setting. The setting for the force field, simulation parameters and output options are set up after the solder atoms, and nanoparticles have existed. The command pair_coeff is used to set up the force field coefficient for each interaction of atoms. Next, the simulation parameters are set up with command neighbor followed by a distance beyond the cut off and the style which is binary. Another command used is the neighbour_modify which affected the building of solder paste environment. The min_style command is used to do minimization for the simulation. For this simulation, the minimization style used is the conjugated gradient. Then, the fix command is used to set the boundary conditions, time integration, and diagnostic options. For computation purpose, the command compute and variable are used in this simulation. Command compute is used to calculate the required value such as the temperature and energy and the variable command is the command to set up the temperature, volume, pressure and some other variables according to the reflow stage environment. The temperature will be set at different temperature to see the different nanoparticles trajectory in the solder. In this simulation, the temperature is set up as 30°C (room temperature), 150°C (ramping temperature), and 250°C (reflow temperature). For the output option, the thermo and dump command is used in this simulation model. This command is used to ensure, the simulation model can be shown in the visualization tools.

Last but not least, the run a simulation part, the run command is used to run the calculation for the simulation model via command prompt. Then, the new file has existed in the directory, which is the dump file. The dump file can show the simulation's image or video via visualization tools.

3 Results

3.1 Molecular dynamics simulation of nano-reinforced solder paste

The molecular dynamics simulation was applied to investigate the nanoparticles trajectory in the lead-free solder paste according to the reflow zone temperature. In this 3D simulation model, the nanoparticles are introduced in a spherical shape and as agglomerated atoms while the solder atoms are introduced as a bunch of single atoms that are freely moved. The color of solder and nanoparticles atoms also represented differently to show clearly the movement of each atom as in Fig.1. The agglomerated, purple color atoms show the Cu nanoparticles,
the red color atoms show the solder atoms while the yellow color in Fig.2, Fig. 4. and Fig. 6. shows the atoms trajectory in the solder in 2D.

Before the reflow phase, which is the main phase in reflow soldering process, there are several stages that occurred first including the preheating, ramping and soaking which has increased the solder temperature from room temperature which is about 30°C, to the reflow temperature of about 250°C. The velocity is added to all atoms as to simulate the increment of the temperature and thus make sure the atoms are not in the static condition. This shows that the thermophoresis-effect occurred.

Fig. 1. Solder paste with doped nanoparticles.

Fig. 2. Solder paste with doped nanoparticles with the mark of trajectory at temperature of 30°C.
Fig. 3. Images of the position of the nanoparticles in the solder paste model at temperature of 30°C at a) 0 second, b) 10 seconds and c) 20 seconds in the x-y plane.

Fig. 4. Solder paste with doped nanoparticles with the mark of trajectory at temperature of 150°C.
**Fig. 5.** Images of the position of the nanoparticles in the solder paste model at temperature of 150°C at a) 0 second, b) 10 seconds and c) 20 seconds in the x-y plane.

**Fig. 6.** Solder paste with doped nanoparticles with the mark of trajectory at temperature of 250°C.
Fig. 7. Images of the position of the nanoparticles in the solder paste model at temperature of 250°C at a) 0 second, b) 10 seconds and c) 20 seconds in the x-y plane.

As shown in the Fig. 3., Fig. 5. and Fig. 7 a),b) and c) the position of the nanoparticles has changed compared to the original position at 0 second at all temperature. This shows that the nanoparticles has moved within the timestep. The collision of the fast moving atoms with the nanoparticles causing the random movement of the nanoparticles which called the Brownian motion.

4 Conclusion

The focus of this paper is to emphasize the steps to simulate the trajectory of the nanoparticles in the solder paste at different solder temperature and it is shown clearly with the use of LAMMPS software as the software focused on the simulation in the atomic scale. The nanoparticles moved according to the temperature in random directions. The most vigorous movement of nanoparticles is shown at the temperature of 250°C while the least vigorous movement is shown at room temperature of solder which is at 30°C.

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