

Investigation of Nano-Reinforced Lead-Free Solder During Reflow Soldering-A Molecular Dynamic Approach



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ABSTRACT

The reinforcement of nanoparticles into the lead-free solder is proved to give good increment in the result of the importance solder properties which includes wetting properties and mechanical properties. This study proposed the new simulation method for the nano-reinforced solder to investigate the complexity and atomic behaviour briefly. The objective of this study is to clearly show the movement of the reinforced nanoparticles in the solder during the reflow soldering process via molecular dynamics (MD) simulation. In this work, Nickel (Ni) nanoparticles will be added into the pure Tin (Sn) lead-free solder. The MD simulation of Ni-reinforced solder at the temperature of 250 °C (reflow phase) was conducted via Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software. This simulation model able to track the nanoparticles movement in the solder during the reflow soldering process. The experimental procedure of 0.01 wt.% Ni nanoparticle reinforcement in Sn100C was also carried out to validate the simulation result. The synchrotron micro-XRF mapping showed the Ni element was agglomerated and thus validated the simulation result. The measured area of agglomerated Ni A in the simulation and experimental results are 1.1708 Å² and 0.9996 Å², respectively. Meanwhile, the result obtained for area B is 0.7696 Å² and 0.6796 Å², respectively. Therefore, the percentage error of simulation and experimental results for both areas of A and B is 10.82% and 13.24%, respectively.

Keywords:

Molecular dynamic (MD) simulation;
nanoparticles; reflow soldering process

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1. Introduction

The growing of Surface-Mount Technology (SMT) due to the increase of the customer requirement for electrical and electronic appliances. SMT has existed in the mid of 1960s [1]. Before the rose of the SMT, the Through Hole Technology (THT) was used to place the electronic components on the circuit board. But, due to the higher cost of drilling as the holes are very small of about 0.1 inches, thus the interest in SMT has increased briskly. The increase in SMT evolution is caused by its

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versatility of soldering and cost-effectiveness which increase the level of performance for the small-scale or large-scale manufacturing processes [2].

Reflow soldering involves four phases which are preheating, soaking, reflow and cooling which have different temperature ranges [3]. Reflow soldering process started with the preheating phase, where the temperature was increased from room temperature (30 °C) to 150 °C. In the next phase of soaking, the temperature was held for a while at the temperature of 150 °C and then rammed up to the next phase. Next, the vital phase known as reflow phase, where the temperature was again rammed up to the peak temperature of 250 °C. This phase allowed the solder to fully wet the substrate. Lastly, the cooling phase where the solder was cooled down to room temperature and solidified.

The use of solder with lead content is banned in electronic mounting technology in the EU because of its toxicity that harmful to the environment. Researchers found that it is difficult to determine the best replacement of Sn-Pb solder that meet the requirement of electronic packaging industries. The alternatives for this problem has been revealed by several researchers which stating that Sn-Ag-Cu [4-5], Sn-Cu-Ni [6] and Sn-Cu [7] solder can be the best settlement to substitute the toxic Pb containing solder. Sn has less vapor pressure and less in toxic, thus still acceptable to be included in the solder paste content [8].

The reinforcement of solder is proven to enhance the quality of solder mechanically, thermally and its wetting properties depending on the reinforced materials. Research on the nano-reinforced solder became more vigorous as researchers found out that adding nanoparticles such as cobalt [1], copper [9-11], silver [12], nickel [13-15], diamond [3], the molecule of iron nickel oxide [16], iron oxide [17], titanium dioxide [18], zinc oxide [19] and others to the solder proven to increase the solder properties in terms of either one, mechanical, thermal, wetting and intermetallic compound layer or all of them. Researchers have also added rare earth elements such as Erbium (Er) [20], Cerium (Ce), and Lanthanum (La) [21], into the SAC solder. They found that a proper weightage percentage of 0.05wt.% to 0.25wt.%, the mechanical strength, creep rupture life, elongation and wettability were improved. Moreover, the carbon nanotubes reinforced in the lead and lead-free solder in many studies and it is proven that the tensile properties [22], microhardness [22-23], shear strength [23,24], and yield strength [25] of the composite solders were improved when added according to optimum composition.

Numerical approaches are introduced in the SMT field to reduce both cost and time-consuming of experimental work. This approaches also demonstrating the reaction of the solder in a particular condition, clearly and accurately. Over the years, there are lots of numerical approaches used to simulate the reflow soldering process, including Finite Element Method (FEM) [26], Finite Volume Method (FVM) [27], Lattice Boltzmann Method (LBM) [28], Discrete Phase Method (DPM) [29] and Molecular Dynamics (MD) [30].

Molecular dynamics (MD) is a method to investigate the analysis of atom location in particular space. MD can also provide information on the molecule properties of thermodynamic and dynamic [31]. Routinely, the MD was used for modeling the time-dependent motions (trajectories) of particles. The forces acting on the particles were measured as derivatives of potentials in conventional implementations of MD. These forces are substituted into Newton's equations of motion, which were iteratively solved for every particle in the system [32]. MD simulated the natural movement of the molecular structure. The energy provided in the MD procedure allowed the atoms to move and collide with the neighboring atoms. The molecule able to cross the energy barriers, in which local minima was separated on the conformational potential energy surface for that molecule, only if sufficient thermal energy is provided [33]. MD simulation demonstrated the behaviour of the atoms and molecules of solder and how they interact during the process [34].

In this paper, the trajectories of Ni nanoparticles in the solder paste at the reflow phase is shown via MD simulation. This study is carried out due to no available study on the simulation work of the molecular dynamics (MD) method of Ni reinforced solder in reflow soldering process.

2. Methodology

2.1 MD Simulation via LAMMPS

There are a lot of software package for MD simulation, including Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [35], Chemistry at Harvard Macromolecular Mechanics (CHARMM) [36], Groningen Machine for Chemical Simulations (GROMACS) [37], Nanoscale Molecular Dynamics (NAMD) [38], Assisted Model Building with Energy Refinement (AMBER) [39], Desmond [40], Tinker [40], DL_POLY [41] and others which can be used subjected to the simulation result needed. LAMMPS software by Sandia National Laboratories was applied 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 also used neighbour lists or known as Verlet lists to keep track of nearby particles. In this case, the commands in the input script (text file) as written in Notepad++ is read by LAMMPS. To perform LAMMPS simulation, the input script is read through the command prompt application which is the command line interpreter. Ovito is used as the visualization tool to show the trajectory of the nanoparticles in the solder.

2.1.1 Simulation setup

To simplify the model, only 3 atoms were involved in this simulation model. For the geometry setup, the composite solder system was modelled by suspending Ni nanoparticles in the composition of Sn and Cu atoms. In the geometry setup, Sn and Cu atoms were arranged in a face-centered cubic (FCC). The molecular weight of Sn, Cu and Ni are 118.71 g/mol, 63.55 g/mol, and 58.693 g/mol, respectively.

The actual input for MD simulation is inter-atomic potential. In the Sn-Cu-Ni system, six interactions were prepared, namely Sn-Sn, Cu-Cu, Ni-Ni, Sn-Cu, Sn-Ni, and Cu-Ni. Lennard-Jones (L-J) potential was used to describe the inter-atomic interactions between the atoms. In order to obtain the value of L-J potential parameters for Sn-Cu, Sn-Ni, and Cu-Ni, the cross-interaction potential was calculated using Lorentz Berthelot (LB) mixing rule [42] which define by:

$$\epsilon_{i-j} = \sqrt{\epsilon_{i-i} * \epsilon_{j-j}} \quad (1)$$

and

$$\sigma_{i-j} = \frac{\sigma_{i-i} + \sigma_{j-j}}{2} \quad (2)$$

where ϵ_{i-j} and σ_{i-j} referred to L-J potential parameters for the interaction between atoms i and j .

The initial geometry setup may produce a poor result with higher energy and the MD integrator may fail if there is atoms or molecules with a larger force in the simulation. Thus, energy minimization is required to optimize the system with lower energy. In this study, the maximum number of iterations and total force evaluation was set at 10000. Transient/unsteady was considered in this simulation.

Next, atomic velocity initialization was set up by assigning random initial velocities to the atoms. The initial velocities assigned for the systems were 1000 m/s, 5000 m/s and 10000 m/s. The initial configurations of the systems did not represent the state of equilibrium. Thus, the equilibration process was performed at a certain time to relax from initial configurations to the equilibrium state before producing data. In this simulation work, the system was equilibrated for 10000 time-steps under canonical ensemble (NVT). The time step of $\Delta t=4$ femtoseconds was used in this simulation.

2.1.2 Input script

Four steps that must be included in the input script which are initialization, atom definition, settings, and run a simulation [30]. In the initialization part, the parameters for the simulation were set up. Commands such as “units”, “boundary”, and “atom_style” expressed the parameters. The second part is the atom definition, where geometry and atoms for the simulation model were created. The commands such as “lattice”, “region”, “create_box”, and “create_atoms” were applied. For the third part, the setting for force field, simulation parameters and output options were set up after solder atoms, and nanoparticles existed. The command “pair_coeff” was used to set up the force field coefficient for each interaction of atoms. Hence, L-J potential parameters were assigned. The last part of run a simulation, the “run” command was selected 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 contained the simulation's image or video via visualization tools.

3. Results

3.1 Sn, Cu and Ni Configuration

There are three atoms involved in this simulation model. Sn atoms represented the solder, Cu atoms represented the atom from the Cu-substrate; and Ni atoms represented the nanoparticles. In this 3D simulation model, the Ni nanoparticles were introduced in the spherical shape and as agglomerated atoms, while solder atoms and Cu atoms were introduced as a bunch of atoms that freely moved, as shown in Figure 1.

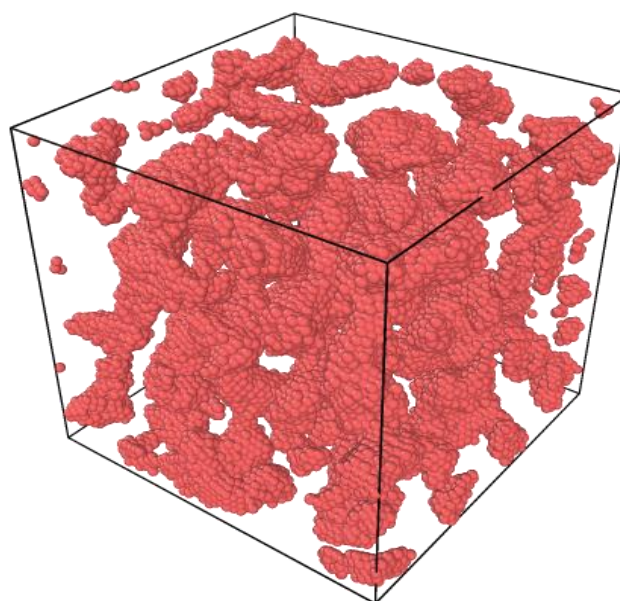


Fig. 1. 3D image of Sn solder with Ni reinforcement

The colour of solder and nanoparticle atoms were also represented differently to show the movement of each atom. The agglomerated of white coloured atoms indicated as Ni nanoparticles, red coloured atoms indicated as Sn atoms and blue coloured atoms as Cu atoms. Both Ni nanoparticles and Cu atoms are in the middle of the model and was crowded by Sn atoms, as shown in Figure 2.

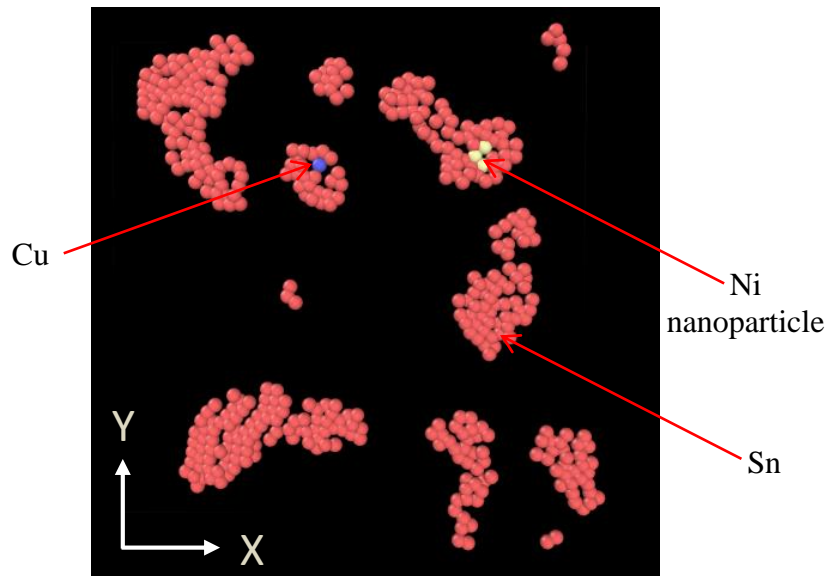


Fig. 2. The sliced image of solder reinforced with Ni nanoparticles in x-y plane with a slab width value of 1 Angstrom with the distance of 10 Angstrom from the normal z-direction

With influence of Brownian and Van der Waals forces, all atoms tend to aggregate to minimize the surface energy. The Cu atoms and Ni nanoparticles were surrounded by Sn atoms, as shown in Figure 2. The aggregation of all atoms in the simulation model led to thermal conductivity improvement. The heat transfer occurred at the surface of the particle. The nano-sized particle itself has a larger surface area, and thus the capability of heat transfer improved.

3.2 Ni Trajectories

Trajectories of the Ni nanoparticles being doped, as shown in Figure 3. The blue colour referred as Cu atoms, white colour referred as Ni nanoparticle, and yellow lines indicated as trajectory line. The directions of the Ni nanoparticles also were symbolized with the arrow of each different Ni atoms namely of 1, 2, 3 and 4. The thermophoresis effect occurred when different type of particles revealed different responses subjected to the temperature. The temperature plays the important role as this simulation model is a dynamic system where the nanoparticles are constantly in motion. This phenomenon is known as Brownian motion, which the nanoparticle absorbed the heat and moved to a greater distance and released the thermal energy to the colder region. The trajectory direction of the Ni nanoparticles at 250 °C showed a chaotic behaviour due to kinetic energy in the system. The zig-zag movement of each particle caused the fibrously identical trajectories line.

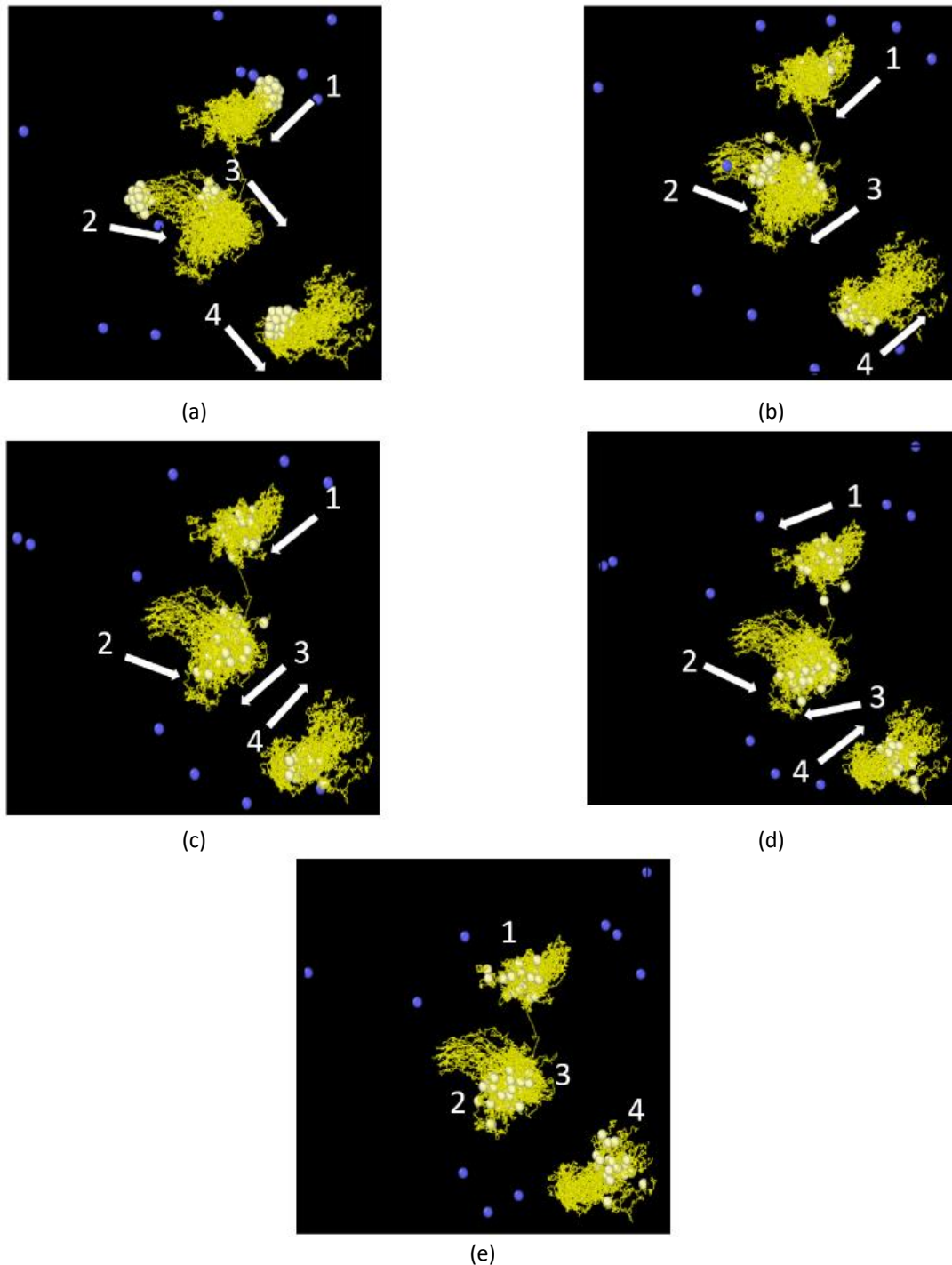


Fig. 3. Images of the position, trajectory and the direction of Ni nanoparticles in the simulation model at temperature of 250 °C at (a) Initial frame, (b) 100th frame, (c) 200th frame, (d) 300th frame and (e) final frame in the x-y plane

3.3 Simulation Validation

The experimental and microstructural visualization procedure of reflow soldering process for 0.01 wt.% Ni nanoparticle reinforcement in Sn100C was carried out to validate the simulation result. At 500th frame of the final frame, the image of the model simulated at 250 °C was taken. For the experimental result, the image of synchrotron micro-XRF mapping of the Ni element distribution in

the soldered sample was obtained. Both simulation and experimental results were then compared, as summarized in Figure 4.

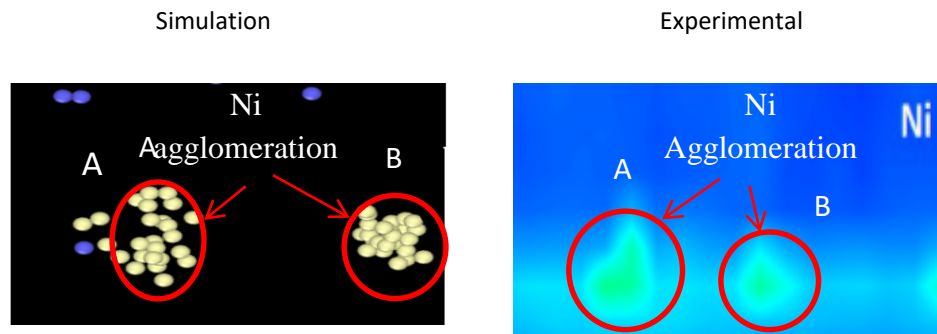


Fig. 4. Comparison between simulation and experimental result

It was found that Ni nanoparticles for both simulation and experimental showed agglomeration behaviour. The simulation findings were proved through the calculation of the agglomerated area of Ni nanoparticles of both simulation and experimental. It was discovered that the size of Ni nanoparticles in the A area is 1.1708 \AA^2 and 0.9996 \AA^2 , respectively, and the percentage discrepancy obtained between simulation and experiment is 10.82%. The agglomerated area of Ni nanoparticles in the B area was also found in the acceptance range. The area for both simulation and experimental results are 0.7696 \AA^2 and 0.6796 \AA^2 , respectively. This value obtained proved the discrepancy of 13.24%.

4. Conclusions

Nano-reinforcement in solder has emerged as a potential alternative in enhancing the quality of the lead-free solder in terms of mechanical and physical properties. The focus of this paper is to show how the simulation of the nano-reinforced solder via LAMMPS software. The result showed the nanoparticles trajected in random directions and moved vigorously at reflow temperature which is the peak temperature ($250 \text{ }^\circ\text{C}$) in the reflow soldering process. This simulation result obtained was then compared with the experimental result of 0.01 wt.% of Ni added in Sn100C solder. Thus, the simulation result was validated where the Ni nanoparticles in the solder are accumulated and agglomerating. In future work, the author will present the trajectory Ni nanoparticle at different solder temperature.

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References

- [1] Tay, S. L., A. S. M. A. Haseeb, and Johan Mohd Rafie. "Effect of addition Cobalt nanoparticles on Sn-Ag-Cu lead-free solder." In *2010 12th Electronics Packaging Technology Conference*, pp. 433-436. IEEE, 2010.
<https://doi.org/10.1109/EPTC.2010.5702678>
- [2] Vianco, P. T., and Y. Feng. "Electronic Packaging: Solder Mounting Technologies." (2016).
<https://doi.org/10.1016/B978-0-12-803581-8.10099-2>
- [3] Chellvarajoo, Srivalli, M. Z. Abdullah, and C. Y. Khor. "Effects of diamond nanoparticles reinforcement into lead-free Sn-3.0 Ag-0.5 Cu solder pastes on microstructure and mechanical properties after reflow soldering process." *Materials & Design* 82 (2015): 206-215.

- <https://doi.org/10.1016/j.matdes.2015.05.065>
- [4] Cheng, Shunfeng, Chien-Ming Huang, and Michael Pecht. "A review of lead-free solders for electronics applications." *Microelectronics Reliability* 75 (2017): 77-95.
<https://doi.org/10.1016/j.microrel.2017.06.016>
- [5] Ma, Hongtao, and Jeffrey C. Suhling. "A review of mechanical properties of lead-free solders for electronic packaging." *Journal of materials science* 44, no. 5 (2009): 1141-1158.
<https://doi.org/10.1007/s10853-008-3125-9>
- [6] Weng, Wayne Ng Chee. "Evolution of Pb-free solders." *Recent Progress in Soldering Materials* (2017): 91.
<https://doi.org/10.5772/intechopen.69553>
- [7] Alam, M. E., S. M. L. Nai, and M. Gupta. "Development of high strength Sn–Cu solder using copper particles at nanolength scale." *Journal of Alloys and Compounds* 476, no. 1-2 (2009): 199-206.
<https://doi.org/10.1016/j.jallcom.2008.09.061>
- [8] T. R. Bieler and T. Lee. (2010). *Lead-free Solder*. Encyclopedia of Materials: Science and Technology (Second Edition) Eds. Oxford: Elsevier, Page 1–12.
<https://doi.org/10.1016/B978-008043152-9.02239-9>
- [9] Shang, Shengyan, Yanfeng Wang, Yunpeng Wang, Haitao Ma, and Anil Kunwar. "Enhancement of hardness of bulk solder by doping Cu nanoparticles at the interface of Sn/Cu solder joint." *Microelectronic Engineering* 208 (2019): 47-53.
<https://doi.org/10.1016/j.mee.2019.01.009>
- [10] Liu, Ping, Xiaolong Gu, Haifeng Fu, and Yang Liu. "The effects of Cu nanoparticles addition in Sn-3.0 Ag-0.5 Cu solder paste on the microstructure and shear strength of the solder joints." In *2016 17th International Conference on Electronic Packaging Technology (ICEPT)*, pp. 852-855. IEEE, 2016.
<https://doi.org/10.1109/ICEPT.2016.7583264>
- [11] Nadia, Aemi, and A. S. M. A. Haseeb. "Understanding the effects of addition of copper nanoparticles to Sn-3.5 Ag solder." *Soldering & surface mount technology* 23, no. 2 (2011): 68-74.
<https://doi.org/10.1108/09540911111120131>
- [12] Bukat, Krystyna, Marek Kościelski, Janusz Sitek, Małgorzata Jakubowska, and Anna Młodziak. "Silver nanoparticles effect on the wettability of Sn-Ag-Cu solder pastes and solder joints microstructure on copper." *Soldering & Surface Mount Technology* 23, no. 3 (2012): 150-160.
<https://doi.org/10.1108/09540911111146908>
- [13] El-Daly, A. A., A. M. El-Taher, and T. R. Dalloul. "Enhanced ductility and mechanical strength of Ni-doped Sn–3.0 Ag–0.5 Cu lead-free solders." *Materials & Design* 55 (2014): 309-318.
<https://doi.org/10.1016/j.matdes.2013.10.009>
- [14] Yakymovych, A., Yu Plevachuk, V. Sklyarchuk, B. Sokoliuk, T. Galya, and H. Ipser. "Microstructure and electro-physical properties of Sn-3.0 Ag-0.5 Cu nanocomposite solder reinforced with Ni nanoparticles in the melting-solidification temperature range." *Journal of Phase Equilibria and Diffusion* 38, no. 3 (2017): 217-222.
<https://doi.org/10.1007/s11669-017-0532-0>
- [15] Tao, Q. B., L. Benabou, L. Vivet, V. N. Le, and F. B. Ouedzou. "Effect of Ni and Sb additions and testing conditions on the mechanical properties and microstructures of lead-free solder joints." *Materials Science and Engineering: A* 669 (2016): 403-416.
<https://doi.org/10.1016/j.msea.2016.05.102>
- [16] Chellvarajoo, Srivalli, M. Z. Abdullah, and Z. Samsudin. "Effects of Fe₂NiO₄ nanoparticles addition into lead free Sn–3.0 Ag–0.5 Cu solder pastes on microstructure and mechanical properties after reflow soldering process." *Materials & Design* 67 (2015): 197-208.
<https://doi.org/10.1016/j.matdes.2014.11.025>
- [17] Gu, Yue, Xiuchen Zhao, Yi Li, Ying Liu, Yong Wang, and Zhenyu Li. "Effect of nano-Fe₂O₃ additions on wettability and interfacial intermetallic growth of low-Ag content Sn–Ag–Cu solders on Cu substrates." *Journal of Alloys and Compounds* 627 (2015): 39-47.
<https://doi.org/10.1016/j.jallcom.2014.12.024>
- [18] Haslinda, M. S., Aizat Abas, F. Che Ani, Azman Jalar, A. A. Saad, and Mohd Zulkifly Abdullah. "Discrete phase method particle simulation of ultra-fine package assembly with SAC305-TiO₂ nano-reinforced lead free solder at different weighted percentages." *Microelectronics Reliability* 79 (2017): 336-351.
<https://doi.org/10.1016/j.microrel.2017.07.054>
- [19] Kanlayasiri, Kannachai, and Nadee Meesathien. "Effects of zinc oxide nanoparticles on properties of SAC0307 lead-free solder paste." *Advances in Materials Science and Engineering* 2018 (2018).
<https://doi.org/10.1155/2018/3750742>
- [20] Shi, Yaowu, Jun Tian, Hu Hao, Zhidong Xia, Yongping Lei, and Fu Guo. "Effects of small amount addition of rare earth

- Er on microstructure and property of SnAgCu solder." *Journal of Alloys and Compounds* 453, no. 1-2 (2008): 180-184.
<https://doi.org/10.1016/j.jallcom.2006.11.165>
- [21] Yu, D. Q., J. Zhao, and L. Wang. "Improvement on the microstructure stability, mechanical and wetting properties of Sn–Ag–Cu lead-free solder with the addition of rare earth elements." *Journal of alloys and compounds* 376, no. 1-2 (2004): 170-175.
<https://doi.org/10.1016/j.jallcom.2004.01.012>
- [22] Kumar, K. Mohan, V. Kripesh, Lu Shen, and Andrew AO Tay. "Study on the microstructure and mechanical properties of a novel SWCNT-reinforced solder alloy for ultra-fine pitch applications." *Thin Solid Films* 504, no. 1-2 (2006): 371-378.
<https://doi.org/10.1016/j.tsf.2005.09.072>
- [23] Xu, Sha, Yan Cheong Chan, Kaili Zhang, and K. C. Yung. "Interfacial intermetallic growth and mechanical properties of carbon nanotubes reinforced Sn₃. 5Ag₀. 5Cu solder joint under current stressing." *Journal of alloys and compounds* 595 (2014): 92-102.
<https://doi.org/10.1016/j.jallcom.2014.01.083>
- [24] Yang, Li, Haixiang Liu, Yaocheng Zhang, and Huakuan Yu. "Study on the reliability of carbon nanotube-reinforced Sn-58Bi lead-free solder joints." *Journal of Materials Engineering and Performance* 26, no. 12 (2017): 6028-6036.
<https://doi.org/10.1007/s11665-017-3033-8>
- [25] Nai, S. M. L., J. Wei, and M. Gupta. "Improving the performance of lead-free solder reinforced with multi-walled carbon nanotubes." *Materials Science and Engineering: A* 423, no. 1-2 (2006): 166-169.
<https://doi.org/10.1016/j.msea.2005.10.072>
- [26] Ghosh, Rituparna, Anwesa Kanjilal, and Praveen Kumar. "Effect of type of thermo-mechanical excursion on growth of interfacial intermetallic compounds in Cu/Sn-Ag-Cu solder joints." *Microelectronics Reliability* 74 (2017): 44-51.
<https://doi.org/10.1016/j.microrel.2017.05.011>
- [27] Salleh, MAA Mohd, S. D. McDonald, C. M. Gourlay, H. Yasuda, and Kazuhiro Nogita. "Suppression of Cu₆Sn₅ in TiO₂ reinforced solder joints after multiple reflow cycles." *Materials & Design* 108 (2016): 418-428.
<https://doi.org/10.1016/j.matdes.2016.06.121>
- [28] Abas, Aizat, Z. L. Gan, M. H. H. Ishak, M. Z. Abdullah, and Soon Fuat Khor. "Lattice Boltzmann method of different BGA orientations on I-type dispensing method." *PloS one* 11, no. 7 (2016): e0159357.
<https://doi.org/10.1371/journal.pone.0159357>
- [29] Haslinda, M. S., Aizat Abas, F. Che Ani, Azman Jalar, A. A. Saad, and Mohd Zulkifly Abdullah. "Discrete phase method particle simulation of ultra-fine package assembly with SAC305-TiO₂ nano-reinforced lead free solder at different weighted percentages." *Microelectronics Reliability* 79 (2017): 336-351.
<https://doi.org/10.1016/j.microrel.2017.07.054>
- [30] Sahrudin, Intan Norshalina, Mohd Shahrizal Abdul Aziz, Mohd Zulkifly Abdullah, and Mohd Arif Anuar Mohd Salleh. "Molecular dynamics simulation of the nano-reinforced lead-free solder at different reflow soldering process temperature." In *IOP Conference Series: Materials Science and Engineering*, vol. 701, no. 1, p. 012014. IOP Publishing, 2019.
<https://doi.org/10.1088/1757-899X/701/1/012014>
- [31] J. Polanski. (2009). 4.14 - *Cheminformatics*, Eds. Oxford: Elsevier, Page 459–506.
<https://doi.org/10.1016/B978-044452701-1.00006-5>
- [32] Krokhotin, Andrey, and Nikolay V. Dokholyan. "Computational methods toward accurate RNA structure prediction using coarse-grained and all-atom models." In *Methods in Enzymology*, vol. 553, pp. 65-89. Academic Press, 2015.
<https://doi.org/10.1016/bs.mie.2014.10.052>
- [33] Pitman, Melissa R., and R. Ian Menz. "Methods for protein homology modelling." In *Applied Mycology and Biotechnology*, vol. 6, pp. 37-59. Elsevier, 2006.
[https://doi.org/10.1016/S1874-5334\(06\)80005-5](https://doi.org/10.1016/S1874-5334(06)80005-5)
- [34] Sahrudin, Intan Norshalina, Mohd Sharizal Abdul Aziz, Mohd Zulkifly Abdullah, Mohd Arif, and Anuar Mohd Salleh. "Study on the Addition of Nanoparticles in the Lead-free Solder During Reflow Soldering via Numerical Simulation-A Review." *CFD Letters* 12, no. 5 (2020): 111-119.
<https://doi.org/10.37934/cfdl.12.5.111119>
- [35] Dong, Hai, Lianhua Fan, Kyoung-sik Moon, C. P. Wong, and M. I. Baskes. "Molecular dynamics simulation of lead free solder for low temperature reflow applications." In *Proceedings Electronic Components and Technology, 2005. ECTC'05.*, pp. 983-987. IEEE, 2005.
- [36] Ong, Ernest ES, and Jong-Leng Liow. "The temperature-dependent structure, hydrogen bonding and other related dynamic properties of the standard TIP3P and CHARMM-modified TIP3P water models." *Fluid Phase Equilibria* 481 (2019): 55-65.

- <https://doi.org/10.1016/j.fluid.2018.10.016>
- [37] Theng, Soong Guan, Khairulazhar Jumbri, and Mohd Dzul Hakim Wirzal. "Membrane Simulation in Room Temperature Ionic Liquid and Oil using Molecular Dynamics." *Journal of Advanced Research in Fluid Mechanics and Thermal Sciences* 42, no. 1 (2018): 38-45.
- [38] Chen, Junshi, Hong An, Binghui Yan, Weihao Liang, and Xin Liu. "Redesign NAMD Molecular Dynamics Non-Bonded Force-Field on Sunway Manycore Processor." In *2019 IEEE 21st International Conference on High Performance Computing and Communications; IEEE 17th International Conference on Smart City; IEEE 5th International Conference on Data Science and Systems (HPCC/SmartCity/DSS)*, pp. 1257-1265. IEEE, 2019.
<https://doi.org/10.1109/HPCC/SmartCity/DSS.2019.00176>
- [39] Witherspoon, Velencia J., Rocío Mercado, Efreem Braun, Amber Mace, Jonathan Bachman, Jeffrey R. Long, Bernhard Blümich, Berend Smit, and Jeffrey A. Reimer. "Combined Nuclear Magnetic Resonance and Molecular Dynamics Study of Methane Adsorption in M2 (dobdc) Metal–Organic Frameworks." *The Journal of Physical Chemistry C* 123, no. 19 (2019): 12286-12295.
<https://doi.org/10.1021/acs.jpcc.9b01733>
- [40] Yadav, Mahima, and Shikha Khandelwal. "Homology modeling and molecular dynamics simulation study of β carbonic anhydrase of *Ascaris lumbricoides*." *Bioinformatics* 15, no. 8 (2019): 572.
<https://doi.org/10.6026/97320630015572>
- [41] Stalker, Megan R., James Grant, Chin W. Yong, L. A. Ohene-Yeboah, Timothy J. Mays, and Stephen C. Parker. "Molecular simulation of hydrogen storage and transport in cellulose." *Molecular Simulation* (2019): 1-10.
<https://doi.org/10.1080/08927022.2019.1593975>
- [42] D. J. T. M. P. Allen. (1987). *Computer Simulation of Liquids*. Clarendon Press.