International Journal of Engineering & Technology, 7 (4) (2018) 3816-3825

International Journal of Engineering & Technology

Website: www.sciencepubco.com/index.php/IJET
doi: 10.14419/ijet. v7i4.16610
Research paper

Molecular dynamics simulation of welding and joining processes: an overview

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Abstract

Molecular dynamics (MD) is a simulation of physical movements of atoms and molecules in the context of N body simulation. The atoms and molecules are allowed to interact for a period of time, giving a view of the motion of the atoms. Molecular Dynamic (MD) simulation is one of the important methods that can be applied to simulate joining processes at the atomic scale. Nowadays, many investigations had been done in molecular dynamics simulation of various joining processes like diffusion bonding, explosive welding, friction stir welding, linear friction welding, cold welding, nanojoining, thermal bonding, and nanoscale soldering. This paper reviews the findings in the literature up to now in this evolving field, specifically, the experimental details, and the advantages and disadvantages of the various types of welding methods that have been proposed. Moreover, it highlights the big prospect of the molecular dynamics simulation and future directions for further research in the joining process.

Keywords: *Molecular Dynamics Simulation; Joining; Welding; Bonding.*

1. Introduction

Permanent joining of materials has been one of the primary activity in the manufacturing and assembling processes trend [1-2]. Through the century, various techniques had been invented for joining materials, such as diffusion welding/bonding, explosive welding, friction stir welding (FSW), and linear friction welding (LFW), cold welding/nanojoining, thermal bonding, and nanoscale soldering. These welding techniques have been developed to generate the most optimize technique to be applied in industrial manufacturing processes.

Based on these needs of joining materials, industry in various countries spent annually a lot of costs to join the materials, such as the USA that had been spent about $300 billion every year [3]. Hence, experimental works to optimize the process also take a lot of costs, more time, and needs the expertise to get the good results that can be applied in industry. Several parameters of joining processes need to be well understood to achieve a better-joining result, such as temperature, pressure, joining time, tensile behaviour, hardness profile of the joined material, diffusion zone thickness, and so on. Moreover, these joining techniques are depended on the materials to be joined which have different properties and behaviour, so that experiments would take a long journey to provide the most optimize processes to join the materials.

In the late of 1980s, the molecular dynamics (MD) simulation was presented to model the various materials and to investigate the phenomena at atomic-scale, include the joining processes, nanometric cutting, or even the behavior of the cells towards cancer and viruses. The essence of MD simulation method is the solution of the Newtonian equation of motion numerically, which is under the ensemble of atoms [3]. These equations then are numerically integrated for very short time range (2-3fs), and equilibrium of the statistical averages are computed as interim averages through the observation time. Principally, evident knowledge of the electronic ground condition in every system setting is necessary in order to have an appropriate description of the interatomic forces. To allow the study of atomistic simulation practically, a classical or also semi-classical potential from which interatomic forces could be addressed is also required. This interatomic forces could be generated by using a correct empirical potential energy function that include the energy sublimation, lattice constant, elastic constants, compressibility, the state of the equation and the stability of the crystal itself. The development of empirical and semi-empirical for many-body potentials in the very first time was did by Johnson in 1989 [4]. Johnson have proposed the potentials of the alloys models that are Cu, Ag, Au, Ni, Pd, and Pt. The ensembles of atom that most likely used are NVE, NVT, and NPT. Nose Hoover method is employed to control the temperature and pressure at the pre-equilibrium, on-equilibrium, and the post-equilibrium based on these ensembles of atoms. To integrate the Newtonian equation of motion, potential model and atom ensemble, the algorithm is required. The firstly used algorithm is Leap-Frog, and then followed by Verlet and Velocity Verlet algorithm. By this early study on the potential models, ensembles of atoms, and algorithms, most of MD simulations in joining processes, especially in metallic materials, have used this embedded atom method (EAM) as its many-body potential model parameter and Velocity Verlet as its algorithm.

In recent years, the molecular dynamics simulation has been used on the various fields of the material investigation. This method has indicate an increasing potential application for analyzing the behavior of the materials at atomic scale that nowadays cannot rendered by using either other theoretical methods or experimental works. These investigations have proved that MD simulation could appropriately figure out the behaviors and characteristics of the joining process at atomic scale. In addition, to verify the correctness of the molecular dynamics simulation models, the experimental work is necessary. According to the data obtained experimentally, most of the reported work is definitely demonstrated that the temperature and pressure range simulated by MD simulation is have similar value and also have a great deal to the experimental works. After the correct model is obtained, this model then could be addressed to investigate the more various parameters and conditions, so that the experimental work which take a lot of costs could be avoided. Therefore, the use of MD simulation to explain and investigate the behaviors and mechanical properties of joining processes is reasonable. The more detail about this issue is discussed specifically in every joining technique that using MD simulation included in this paper. Furthermore, the aim of this study is to provide an overview of these investigations and to figure out the current state of the research related to the behaviors and mechanical properties of the various materials in the joining processes as well to discuss the future development of the molecular dynamics simulation of the joining process.

2. Application of the molecular dynamics simulation of the joining process

The development of MD simulation on the joining process has been done through the decade and is very clear that it delivering much new understanding on the various joining processes at the nanoscale. The joining quality is determined by the mechanical properties that achieved, which also has been proved by some researcher, could be estimated using MD simulation. Even though that there are some particular problems when the MD simulation is used to investigate the behavior of materials in joining processes, such as the system which is relatively small and lack of information that provide the best parameter of the materials used (the potential model), the potential application of MD simulation is still promising and is indicated by the needs of understanding the behavior of materials in more detail and smaller scale in order to gain the desired quality of joining parameters, especially in the case that the material used is in nano-sized material such as carbon nanotubes and nanowires, which in MD simulation the system is running at the nanometer-sized scale and at femtosecond timed scale. Furthermore, the low-cost research that offered by MD simulation compare to the experimental works has led MD simulation to be used as a most used complementary method to the experimental work.

In this part of the paper, the investigations of MD simulation in various joining processes that have reported by some researcher, including diffusion welding, explosive welding, friction stir welding, linear friction welding, nanojoining/cold welding, thermal bonding, and nanoscale soldering is addressed. Moreover, the mechanical properties, which is inseparable from the joining process itself, also addressed, particularly on the welded material.

2.1. Diffusion welding/bonding

Diffusion welding is a special method that has a feasibility of joining materials whereas the materials has some unique metallurgical characteristic. A sample that to be joined using diffusion welding method must be designed in specific and prepared well in order to get some particular metallurgical characteristics to get a successful joint [5]. Therefore, this technique is required much expertise and takes a lot of time and money which in case of its application in industrial processes should be estimated in detail. But, there are some particular application that the diffusion welding used, especially when some cases are occurring, such as: (1) there are metallurgical problem that needs to be avoided, (2) shares to net dimensions' fabrication, (3) the corrosion resistance that needs to be maintenance using titanium and zirconium, and (4) the fabrication of uniform though-thickness in a thick part, such as titanium laminates. Furthermore, diffusion welding/bonding is involved a high pressure and high temperature which is used to join some advanced materials that cannot be joined by classical methods. Because of this advantage, many researchers have given their attention to the diffusion welding/bonding process.

Meanwhile the investigation of diffusion welding is needs to be done through decade, the MD simulation is coming with some particular benefit, such as the ability to avoid a sample preparation [3] which is takes a lot of cost. One of the very first attempt of MD simulation on joining processes that using diffusion bonding method is employed by Chen et al [3, 6]. In their first model, instead of concern into the two main parameters that involved in diffusion bonding, that is pressure and temperature, they only concern on the influences of pressure, especially on its relationship to the interfacial region thickness. Therefore, in that study they only have figured out that the interfacial region thickness is significantly influenced by the pressure. Meanwhile, as a development of the previous model, Chen et al. [6] built a system of Cu-Al by means of MD simulation. Through their research, they investigated the behaviour of the system at various temperature and also involved surface roughness, instead of only concern on the temperature parameter. The results of this study have shown that the thickness of the interfacial region also depends on the temperature, not only by pressure, as stated in their previous work. It is shown that below the temperature of 750 K, the thickness of the interfacial region is increased in a stepwise, which is of manner as a function of time. After 750 K, the thickness is increased smoothly and rapidly. The model that developed by Chen et al. is shown in Figure 1.

Another researcher also has done the MD simulation on the same material [8, 9]. However, Li et al. [7] have focused on the atmospheric pressure and showed that the Al atoms are harder to diffuse compare to Cu due to different melting points. They also pointed out that the appropriate temperature ranges to perform a diffusion bonding of Cu-Al system is 750-800 K. Meanwhile other research [8] focused on the difference between the surface with and without roughness. The result is the generated grooves by the surface roughness, is mainly filled by the deformation of Al. The diffusion is promoted as the contacting area is increased. Basically, these three researches have a similar finding with the finding of Chen et al. [3, 6].

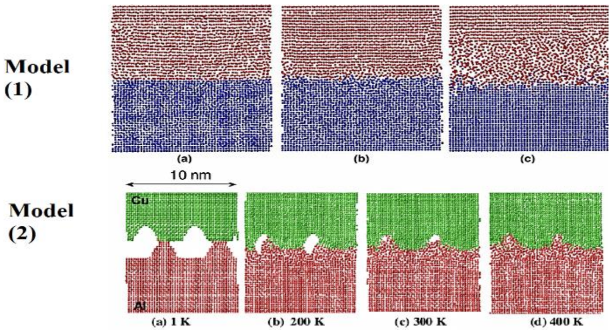

Fig. 1: (Model 1) Cu (Red) and Ag (Blue) System Respectively at Different Pressure after 200 Ps Under 1150 K. (A) 50 Mpa, (B) 100 Mpa, (C) 150 Mpa [3] and (Model 2) Including the Influence of Surface Roughness and Variation of Temperature Under Certain Pressure of 20 Mpa [6].

2.2. Explosive welding

The explosive welding is a solid-state joining technique that involved an extremely high velocity with high explosive energy. It is employ the conversion of kinetic energy into heat that occurs during the explosion at the joint interface [5]. As a well-established method for joining metals, explosive welding has been widely applied in the industrial manufacturing processes for decades. Furthermore, as the explosive welding is performed in a very short-ranged time, it is difficult to figure out all the phenomenon and behaviour that occurs during the process. In this case, same as the diffusion welding/bonding, MD simulation is performed to investigate such behavior at the atomic-scale and to avoid the cost of these joining processes that is relatively high.

In recent years, MD simulation was used to explain these behaviors. As a further explanation to the experiment, Kim et al. [10], have shown the feasibility and good agreement of MD simulation and its experiments in explosive welding. The aim of their study is to explain the mechanism of the evolution and formation of nano-grained tribo-material in high-velocity, especially in its subsurface microstructure characterization. Their simulation shown great agreements to the experiment, that the atomic-scale flow and mixing is contribute to the disordered and nanostructured surface layer. The possibility of using MD simulation as a further explanation to the experimental works is figure out in this study and is also could be used as a basic study which, in some case, could engage another further investigation of the explosive welding process.

Others researcher have investigated the correlation of the local transient melting with the jetting at the interfacial region in explosive welding [11]. Their simulation has indicated that the jet formation is increasingly with fine grain size near the welded interface, and it is filling off the atom layers nearest it, and that has a good agreement with the results of the experiment. Also, in the Cu-Al system, Chen et al. [12] shown that the difference melting points between Cu and Al materials have facilitated the diffusion of Cu atoms and filling it into the Al side which occur under relatively low collision velocity, while Al slab needs higher collision velocity. The transverse velocity affects the diffusion coefficient. Fig. 2 shows the configuration of Cu-Al planes under different velocity after 20ps.

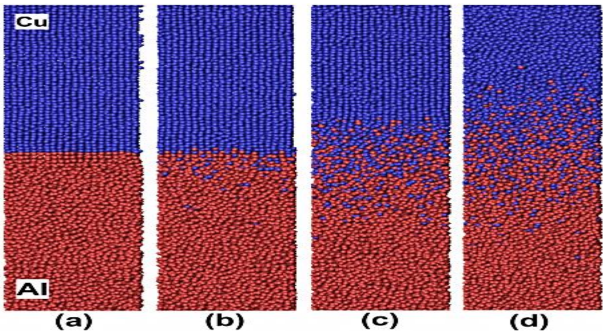

Fig. 2: Snapshot of Configuration of Cu-Al Planes at Different Velocity that are A) 100 M/S, B) 300 M/S, C) 500 M/S, D) 700 M/S at 200 Ps after The Unloading Stage [12].

Others materials, such as Ni50Ti50-Cu, is investigated using molecular dynamics simulation by Chen et al. [13] as a continuation of their previous study. They have concern on the geometrical similarity of atomic concentration distribution in various time. Using this similarity, they have proposed some equation that could estimate the concentration distribution at any time. Also, in this simulation, it has a well similarity to the experimental work. The concentration distribution produced by Chen et al. [13] is shown in Figure 3.

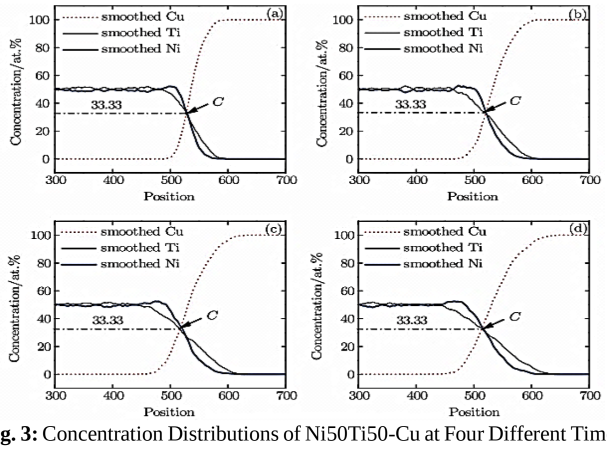

Fig. 3: Concentration Distributions of Ni50Ti50-Cu at Four Different Times: A) 200 Ps, B) 400 Ps, C) 600 Ps, D) 800 Ps [15].

Zhang et al. have performed a molecular dynamics simulation on the explosive welding of Al-Mg system [14]. Instead of concern about the results of their simulation, like Chen et al. [12,13] do in their simulation, Zhang et al. [14] prefer to concern on the diffusion coefficient that affected mainly by collision velocity. Firstly, the diffusion coefficient of the Mg atom is larger than the Al atom, but by increasing the collision velocity, the difference of diffusion coefficient between Mg and Al is decreased.

2.3. Friction stir welding (FSW)

FSW is mainly employ the conversion of mechanical energy into heat at the joint interfaces. The common method used in this technique is to rotate one of the materials to be joined, in this case, the other material is held in a stationary position, meanwhile the rotating materials is given pressure to the held one [5]. This process will give enough friction to produce required heat to deform the interfaces of materials and the joining process then could be produced.

Friction stir welding is a complex joining process, which is used for joint various dimension and shape and involving the not only pressure and temperature but also the rotation speed of tool work. Some recent works on friction stir welding also using MD simulation to explain the behaviour of the material at atomic-scale. Dmietriev et al. have performed a molecular dynamics simulation to study the patterns of microstructure during FSW [15]. They have shown that after the passage of the rotating tools along the boundary, there was a complex configuration comprising the intermix of iron and copper atoms. There are replacements of Cu atoms to the Fe atoms, and vice versa as shown in the detailed analysis of resultant structure. The projection of atoms can be seen in Fig. 4.

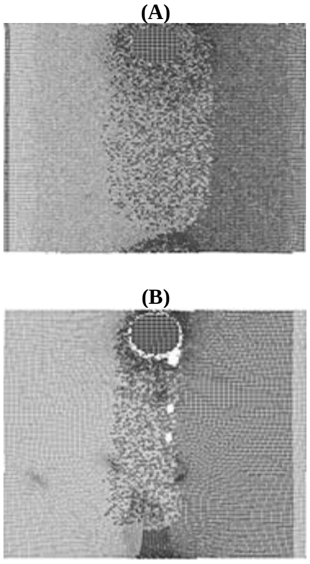

Fig. 4: Projection of Atoms after Passage Tool of Cu-Cu after Different Speeds Tool A) 500 M/S and Ω = 0, 1ps-1 and B) 100 M/S and Ω = 0, 1ps-1[15].

An intensive investigation of FSW using MD simulation also performed by Nikonov et al. [16]. They have modelled the two crystallites of copper, crystallites of copper and iron, and two crystallites of aluminium 2024, which each of it will be simulated to joining using FSW technique. From the process of joining these three crystallites, the simulation results have shown that under a certain condition of loading when tool passes, there is a region where original position of crystal lattice could occupy by the atoms. It is also shown that there is an influence of an additional oscillating impact to the moving tool on the structure of the weld joints.

One of the important phenomena in FSW is mass transfer, who have studied by Konovalenko et al. [17]. The mechanically activated processes are associated inseparably with the intensive generation of discontinuities, mass transfer and structural defect of different scales. They have test two main parameters that involved in FSW, that are the velocity movement and angular velocity of the tool. If the velocity movement is increased and the angular velocity of the tool is decreased, then the penetration depth of atoms into opposite crystalline is reduced. Otherwise, if the angular velocity amplitude of the tool will impact to increase the interpenetration. Nikonov et al. [18] found the similar influence of the vibration amplitude applied to the FSW tool. Beside that finding, as the tool passes along the weld line, the material crystal structure is rearranged and recovered its regular order in subsequent by mixing of their surface atoms. In a further research performed by Konovalenko et al. [19] who have demonstrated that applying the auxiliary vibration action (AVA) to the rotating tools will reduce the tool travel resistance by 15% and the reduction of its growth rate. Thus, they show the feasibility to adjust the FSW process parameters when the auxiliary energy is applied.

2.4. Linear friction welding (LFW)

LFW is an efficient solid-state welding technique which involves the relation of force, heat, and metallurgy. To perform LFW, the two step that involve reciprocal motion and applied pressure is needed. Firstly, the two components/materials need to reciprocate together in different linear direction with certain pressure. This friction process will produce heat for bonding process. When the work pieces are reach particular condition in its metallurgical characteristic that sufficient for bonding process then a certain pressure is applied to the work pieces, and the successful LFW process is performed and a metallurgical bond is created. [22–24]. Although many types of research have been done to investigate the phenomena and properties of LFW, there are some physical phenomena and correlated properties to the atomic diffusion in LFW not observed clearly. The MD simulation then playing an important role in such limitation.

By using molecular dynamics simulation, Jiao et al. [23] have done an intensive investigation of LFW properties, especially on surface roughness and pore parameters of Ni and Al systems. Their simulation results demonstrated the LFW process at atomic scales that involved rough surfaces and pores. During the process, the rough surfaces are gradually flattened and the final weld structure is mainly influenced by the harder material, that in this case is Ni. Meanwhile, in the with pore case, the pore closure is occurring during the LFW process. The Al slab pore closure is promoted by atom diffusion, while the Ni slab is takes place in the step of forging stage, and is mainly influenced by the deformation of the interface of the materials. Fig. 5 show the process and configuration of the Ni-Al system with rough surface and pores.

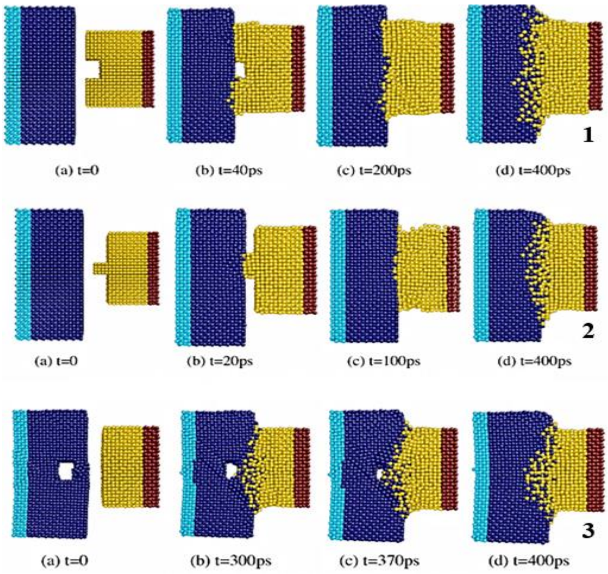

Fig. 5: Process and Configuration of A Cross-Section of LFW: (1) and (2) with Rough Surfaces and (3) with Pores [23].

In different materials, Song et al. [24] have investigated the LFW between dissimilar Ti-based alloy. Their modelled system of Ti-based alloys has been done on rough surfaces. The diffusion behaviour demonstrated by their simulation has shown that the heat produced on the interface of the two rubbing slabs is promoted by friction time, that is rapidly at the beginning and then fluctuated. Moreover, the pressure and reciprocating motion is causing large amounts of atoms were forced out of the interface. It is also shown that the distorted close-packed structure of perfect hexagonal structure and the initial structure gradual deformation on the long-range order is occur during the process. The atomic diffusion behaviour during the process is diverged with direction and Ti atoms have showed higher diffusion coefficient compared to Al atoms, influenced by its melting point. Fig. 6 demonstrated the LFW process at a different time.

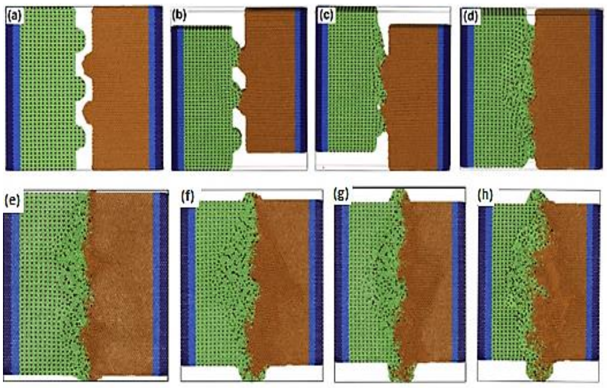

Fig. 6: Simulation of LFW Process with Different Time: A) T = 0 Ps, B) T = 5 Ps, C) 15 Ps, and D) T = 76 Ps, E) T = 200 Ps, F) T = 500 Ps, G) T = 800 Ps, And H) T = 1200 Ps [24].

2.5. Cold welding Nano joining

The cold welding process is involved plastic deformation which causing the generation of a new, clean surface at the joint interface, and similar to the diffusion bonding which is needed a sample preparation, this technique also then promotes a solid-state welding. The cold welding techniques has been used to joint soft and ductile metals in various ranges application [5]. Cold welding is established as a response to the demand of micro or even nanomachining. The nanojoining nowadays playing a very important role to produce a very precise form of joint, such as in carbon nanotubes (CNTs) and Nanowires (NWs) fabrication.

Since MD simulation performs in the nanoscale process, this method is very fit to be used in nanojoining investigation and research. An intensive investigation of joining CNTs was performed by Krasheninnikov et al. [25]. Their study has carried out the possibility of using electron-irradiation to create a molecular junction between CNTs. They have proposed a method that mediated by the dangling bond saturation and also the reconstruction of carbon network that occur near the vacancies in the involved junction created area, in this case, the high temperature and ion irradiation is employed for welding CNTs. It also indicates the influence of high temperature, which is indispensable for this transformation and for defect reinforce far from the junction areas, but the ion irradiation is still required to provide the CNTs welding Meanwhile, an investigation by Jang and Susan [26], instead of using an ion-irradiation, they perform an electron beam irradiation. They found that covalent junction is predicted to form between various types of CNTs that contain many defects. The covalent junction is likely represented the experimentally welded nanotubes under highly non-equilibrium synthesis condition. To join CNTs onto metallic substrate Song et al. [27] simulations indicates the bonding process of CNTs onto metal could be controlled in two ways. Firstly, concentrate the energy to the metal surfaces to promote the surface melting. Secondly, the wetting properties of the substrates should be excellent or if the substrate do not reach the required wetting properties, it could be utilized to enhance the wetting property of the metal substrate atoms to the CNTS surfaces. Through the Ar bombardment, Kucukkal and Stuart [28] have carried out the feasibility of welding CNTs. In their simulation, they consider the influence of involved parameter that promote the welding, that are annealing temperature, particle flux and fluency, nanotubes chirality, and Ar kinetic energy. They have demonstrated the most efficient bombardment condition which are lead to the most weldable condition of the nanotubes with the less loss of graphitic carbon nanotubes properties (i.e. conductive). The mentioned condition is promoted by impact energy at 100 eV which is relatively at mild impact value, with a low particle flux and fluency, but at high temperature that is at 3000 K annealing. They also stated noteworthy for particular experimental application, which is a high junction quality is maintained for a relatively broad range of fluencies, which is from 3.1019 m-2 to at least 1.1020 m-2.

An investigation of patterning via cold welding was performed by Song and Slorovitz [29]. They have found that for small works of adhesion, the mechanism of de-bonds of the film during the stamp retraction is elastically from the substrate before the onset of plastic deformation inside the film. As well, to provide a good measure of the degree of damage induced during the patterning process is promoted by the maximum elastic de-bond length of the film.

Some studies on molecular dynamics simulation also performed to explain the characteristics and properties of cold welding processes of nanowires (NWs). Pereira and da Silva have performed an investigation of the cold welding of Au and Ag NWs [30]. They have found that it is possible to use cold welding in metal NWs due to fact that crystalline structure by breaking can be reconstructed to their face-centred cubic structure during the process. Very few defects were detected for the final cold-welded NWs. Small pressure also needed for the process of cold welding to occur. Fig. 7 has shown the process of Ag-Au cold welding NWs.

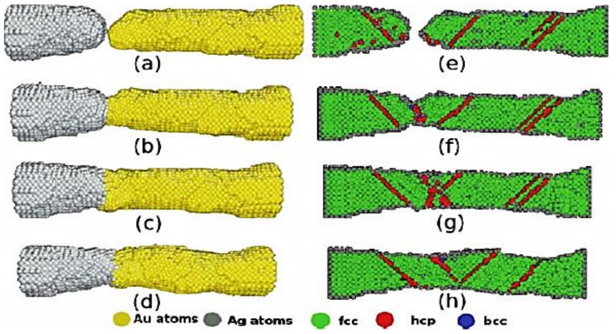

Fig. 7: Welding of Ag-Au Nws. A) Two Tips, Silver (Left) and Gold (Right), before the Welding Process. (B, C) Welding Process. (D) Final Structure. (E-H) Ackland-Jones Analysis of Welding Corresponding to the (A-D) Structures [30].

As a process to understand the tensile behaviour of cold welding experiments, Wang and Yi [31] have performed MD simulation of ultra-thin Au NWs. They found that, for a small NWs of φ3 nm and φ 4 nm diameters, the mechanical properties of single NWs are different and better than welded NWs. The intended properties are Young's modulus, yield strength, and yield strain. Also in ultra-thin Ag, Dai et al. [32] have performed side to side cold welding that is being dominated by atoms kinetic compared to thermodynamics, which provides critical insight into the three-dimensional nano-system integration.

Huang and Wu [33] have employed the welding strength to compare the quality of nanojoining. They conclude the ratio of welding strength of Au and Au welded NWs is better than Ag and Cu welded NWs at room temperature and this is also applies for the welded NWs at the high-temperature range (600 K – 900 K). Further explanation at comparison also performed by Wu et al. [34]. They have found by their MD simulation, that the comparison of Au-Au, Ag-Ag, Au-Ag NWs shown that Au and Au nanowires have the best join quality, meanwhile the dissimilar joining of Au-Ag has the worst. Huang et al. [35] have compared copper NWs with single-crystalline and twinned crystalline structure. It was confirmed that fivefold twinned nanowire (FTNW) has shown increased strength but decreased elastic limit and ductility. The employed strain curve showed that both nanowires could be joined through small loading, but the presence of twin boundaries, that limits the atomic vacancies, leads to higher stress accumulated in FTNW.

An intensive investigation of crossed Ag NWs has done by Cui and Wang [36]. Their finding revealed when the joining temperature is high, the nanostructure of Ag NWs had been significantly deformed into shorter length and larger diameter. Furthermore, it is presenting the uncontrollable melting characteristics based on the chaotic at atomic structure, leads to the conclusion that high temperature is not suitable for joining nanowires. If performed by cold welding, where the temperature is maintained at about 300 K, the Ag nanowires can be contacted partially then the partial mixture of Ag atoms is created. Fig. 8 shows the configuration of crossed Ag NW at 300 K. Meanwhile, between axially positioned Ag NWs, Cui et al. [37] also have performed MD simulation to investigate this phenomenon. Their simulation results showed that the temperature and the distance between Ag NWs in axial direction have a great influence on nanojoining quality. They also found that performing of the nanojoining process at high temperature leads to disordering of the atoms. Furthermore, the atoms queue become to distort strongly on properties of thermodynamic, but weakly on the effect of metal bonds. They demonstrated the difference between using relatively high-temperature welding (~300 K) and cold welding that showed a good junction quality. Fig. 9 shows the configuration of nanojoining of Ag in various temperature while Fig. 10 reveal the configuration of nanojoining of Ag in temperature of 300 K. Another method in nanojoining of Ag NWs, that is using plastic deformation, was demonstrated by Liu et al. [38]. They have found that sufficient plastic deformation is the key to realize a successful welding, especially when the nano-object, such as NWs, have large mismatching orientation. Although the lattice orientation of joint is complex, in contrast with that, no defects were found in experimental or simulation.

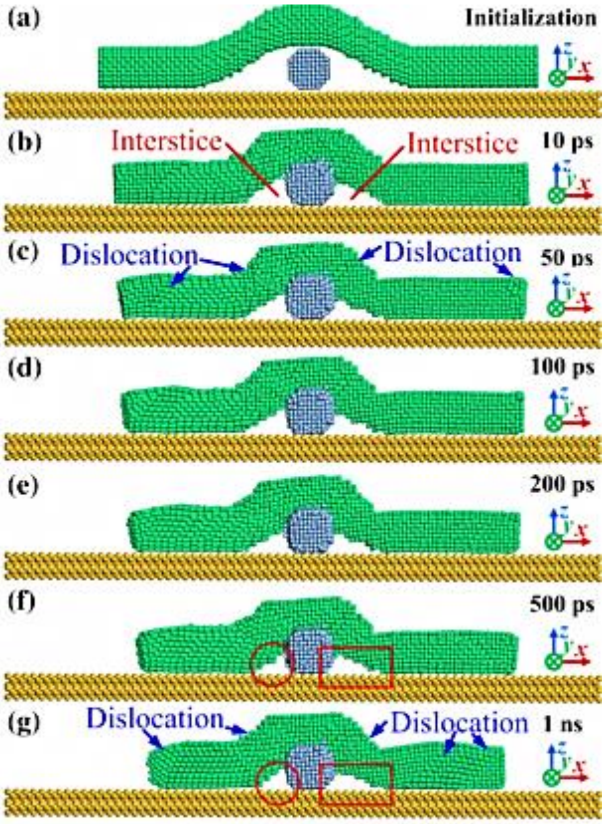

Fig. 8: The Configuration of Crossed Ag NW at 300 K [36].

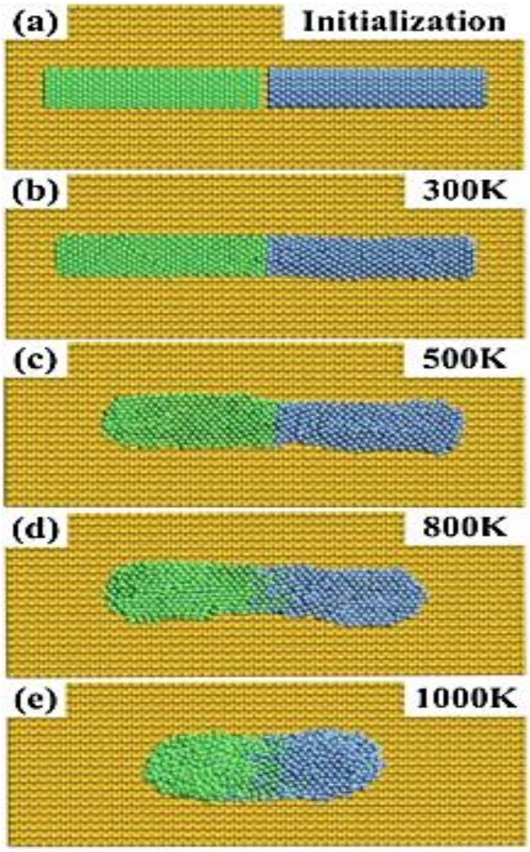

Fig. 9: The Configuration of Ag Nano Joining at Various Temperatures [37].

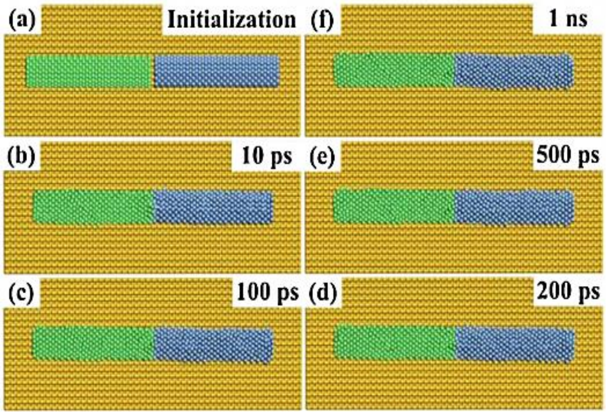

Fig. 10: The Configuration of the Ag Nano joining Process in Temperatures of 300 K [37].

The investigation of the cold welding effect of NWs, such as size [39] and velocity [40] has been concluded that the smaller NWs have better weld strength. The effect of structural instability increased by decreasing NW width, that leads to difficulties in making the alignment. As well, by increasing NWs width, the elongation ability of the two welded NWs also increased. The change of structural stability is caused by the increase of kinetic energy by means of increasing welding velocity. Zhou et al. [41] also showed that the loading time of the velocity could be used to control the number of defects in the welded NWs.

Another effort also performed by Cui et al. to join Ag NWs and single-walled CNTs [42]. They have demonstrated that when the single-walled CNTs and Ag NWs are arranged coaxially at the same diameter, the single-walled CNTs will move into the Ag NWs and then contact with the head of Ag NW. The Ag NWs could be dragged into the CNTs at a relatively low temperature, which will form core filling. Meanwhile, the high temperature, which leads to a similar nano-droplet structure, will not form a core filling. Also, the size is matter as well the arrangement, by means of the single-walled CNTs and Ag NWs needs to be at proper diameter to perform a core filling and should be aligned at axial configuration. Fig. 11 shows the proper process of core filling. An intensive study carried out by Wang and Shin [43] to show the feasibility of joining Cu-Ag core-shell nanoparticles (NPs) and NWs. They have shown that various joining mechanism, such as crystallization-amorphization, reorientation, and Shockley partial dislocation were determined depending on its geometrical configuration. The tensile tests showed that the welded Cu-Ag core-shell have higher rupture strength than the core-shell nanowires itself. They also underlying potentially to achieve using mentioned joining mechanism to get the desirable thermal, electrical, and mechanical properties of joined materials.

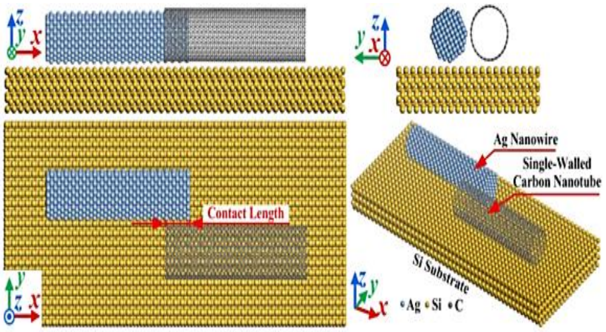

Fig. 11: The Atomic-Scale Configuration of Axial Nanojoining between Ag Nws and Single-Walled Cnts with Side to Side-Structural Style [42].

2.6. Thermal bonding

Thermal bonding is used in joining of polymers, which applied heat and pressure to the surface that will be joined until the bond is formed [44]. The polymer surfaces are brought into close contact and heated above their glass transition temperature, which is the temperature of a polymer that could promote the polymers to be joined. so that it will be allowed to inter-diffuse for a certain welding time [45].

Welding of polymer which has a non-uniform molecular weight had been studied by Prager et al. in 1983 [46]. They have carried out the feasibility of welding a polymer, even with non-uniform molecular weight. Since polymer welding has some complexity, such as its fracture. MD simulation has been used to explain such characteristics since t 1987 by Wool et al. [47]. The aim of their study is to explain the strength of polymer interfaces. There are some complex relationships between structure and strength as revealed by their study, therefore it is a must to use the new entanglement concept, especially in microscopic deformation model. Furthermore, the mechanical properties revealed by this study are related to the structure in the polymer interface and it is used microscopic deformation mechanisms which involving bond rupture and disentanglement. The information of concentration profiles was explained by this research. However, the use of MD simulation wasn't so significant in these decades, limited by the computational machine.

An intensive study conducted by Rottach et al. [48] have shown that the cross-links of the networks, at the first stage, are subsequently removed, while a fraction of the second-stage cross-link contributes to the effective first-stage cross-link density. The reacting networks from the MD simulation is extracted to get the stress transfer fraction, which is have a good agreement with the Flory and Fricker prediction. Also, theoretical transfer function of Fricker which based on the modified slip tube model of Rubinstein and Panyukov is employed to accurately calculate the fractional stress which occur during removal of the first stage of cross-links. An investigation of the dynamics of polymers across an interface was conducted by Pierce et al. [49] which have revealed the motion of the chain ends found to the significantly affect to the interdiffusion across particular interfaces. But, it has a different behavior with the self-diffusion of the polymers, which melts during the early stages of diffusion and it is characterized mainly by the repetition-like chains in a constraining tube formed by neighbouring molecules.

According to the autocorrelation of the function of end-to-end analysis, Yokomizo et al. [50] have revealed that anisotropic motion of chain is have a significant impact to enhance the interfacial thickness and relaxation of the chain orientation. Fig. 12 have shown the typical example of evaluating the thickness of the weld interface. From the motion at the particular involved segment of the interface, the density profile is analyzed at the end and center beads during the diffusion process. It has shown that the interdiffusion of the end segment is faster compare to the center of the segment and is suppressed in the oriented of long chain. Ge et al. [45] have discussed about the strength at the interface of polymers saturation. From the bulk of shear strength, the interfacial strength of polymer is saturated long before the polymer diffusion which revealed by the radius of gyration. The main failure model changes which occur from the chain pullout along with the strength increases at the polymer interface to chain the scission as in the bulk. Furthermore, the increase of the strength of the interface before the saturation is occur is revealed to be proportional to the number of the entanglements of the interface between chains from the contrary sides.

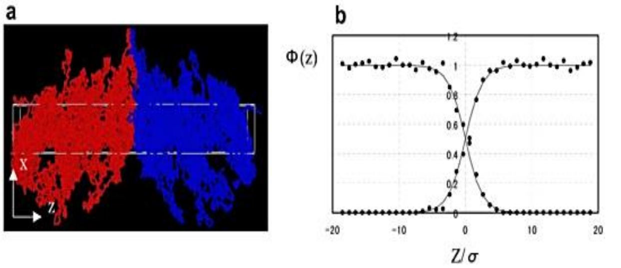

Fig. 12: A) Typical Example to Determine the Thickness of Welded-Polymer Interfaces and B) Corresponding Volume Fraction Profile [50].

Another good attempt have studied by Ge et al. [51] which have carried out the characteristics of tensile fracture of welded polymer interfaces by terms of miscibility, entanglements, and crazing. They have revealed the failure of the bulk polymers which occur during the craze formation, and then followed by the craze breakdown through the chain scission. As the small welded interfaces have not enough strength to support the craze formation, and have also failed at small strain through the interfacial of the chain pullout, they have proposed a method to weld when the chains are formed at an average of about the entanglement across the interface, and then a stable craze is formed. They employ the continuum fracture of the mechanics' model to calculate the interfacial fracture energy by coupling the results of the simulation to such model. Meanwhile, immiscibility limits the inter-diffusion and thus suppresses entanglements at the interface. Small degrees of immiscibility potentially reduce the interfacial entanglement, and that's enough to bring failure occurs by chain pullout. Fig. 13 have visualized the failure of equilibrated immiscible interfaces during tensile tests.

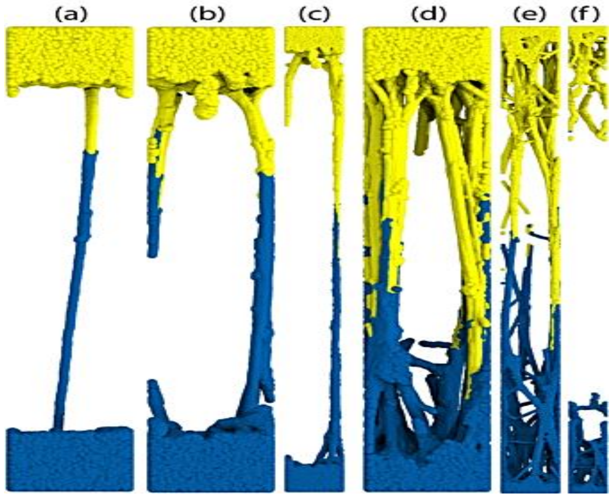

Fig. 13: Failure of Equilibrated Immiscible Interfaces during Tensile Tests [51].

A study on bond exchangeable reactions (BER) has conducted by Yang et al. [52]. They have revealed that the modulus strength and the yield strength is found to be increased in line to the temperature is increases and the elapsed welding time. In some case, the modulus strength and yield strength is reached the same value with the as-received sample. Also, the lower crosslink of density influenced to the shorter welding time and have made the degree of polymerization is lower that led to a slower surface welding between covalent adaptable works. However, the entanglement of the polymer chain would notably reduce the diffusivity. Both Leibrer's theory and Stukalin's theory can predict the penetration depth of the polymer chain, which have a good agreement with their simulation. Fig. 14 shows the structure of the welded polymer, number of BER, and stress-strain.

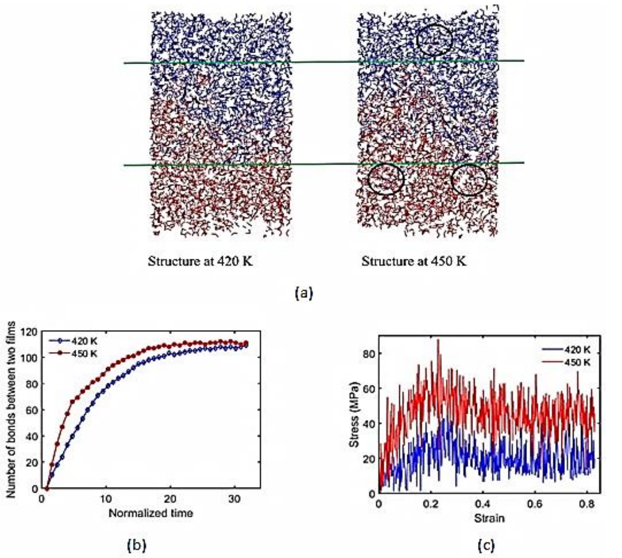

Fig. 14: A) Structure of Welded Polymer; B) Number of BER; and C) the Stress-Strain Curve [52].

2.7. Nanoscale soldering

Soldering is an additive manufacturing process that involved additive material to join one bulk slab with other bulks. This joining process at nanoscale is promoted by the needs of the miniaturization of devices, especially in electronics wire, substrate, and so on. Carbon nanotubes (CNTs) has been one of the one of the promising candidate that could be used as a wire because of its mechanical and electrical properties. The ability to prevent oxidation process also has been the reason why CNTs is used as body-armor of nanomaterials, such as nanowires (NWs). Since the CNTs and NWs are nanoscale materials, MD simulation has been extensively used to explain the behavior and mechanical properties of these materials, include those welded materials behavior and mechanical properties. There are two good attempt that have aim to provide a good explanation of nanoscale soldering, that is to soldering the CNTs and CNTs [53] and iron filled CNTs [54]. Cui et al. [53] use 2 nm silver nanoparticle as an additive material to join a couple of single-walled CNTs. The 2 nm silver nanoparticle is start melted at the temperature of about 605 K. After the silver nanoparticle is melted, the system shown a core-filling process, and this core-filled material is joining between CNTs. This process is shown in Figure 15.

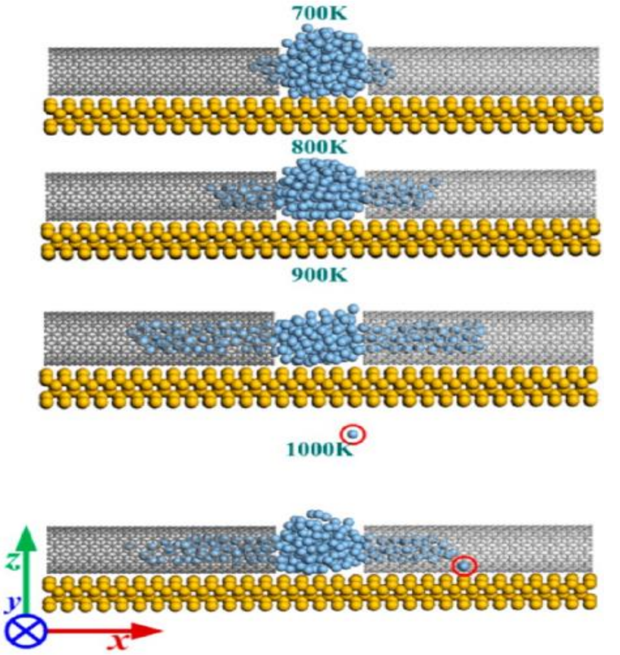

Fig. 15: Core Filling Process of Joining CNTS and CNTS Using Soldering Techniques [53].

An intensive study had been done by Munizaga et al. [54] to solder the iron-filled CNT. This method is doubted to be done by experimental works because of the temperature needed to deform the iron inside the CNTs is too high to be applied experimentally, that is about 1800 K. Even though that it is very difficult to join CNTs with CNTs, this simulation has demonstrated its feasibility to join a core-filled CNTs. The work of Cui et al. [53] was definitely more realistic to be applied, since the temperature range is about 1000 K. The process of soldering the iron-filled CNTs is shown is Figure 16.

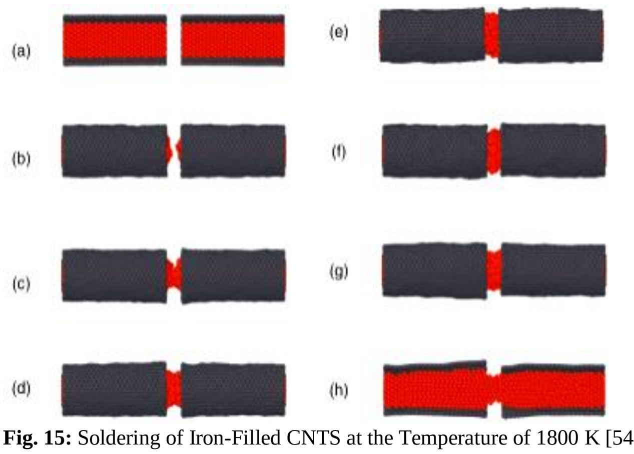

Fig. 15: Soldering of Iron-Filled CNTS at the Temperature of 1800 K [54].

3. Advantages and disadvantages of MD simulation on the joining process

As an alternative method to investigate the behaviour and mechanical properties of the joining process and post-process, MD simulation has some advantages, which are:

1) The main advantages of MD simulation is it's not limited by preparation of the sample and the testing condition and parameters, nevertheless, it still can be used to simulate and investigate some mechanical behaviour in nanoscales [3].
2) The MD simulations offer extensive parametric studies and have potential to avoid the need for long experiments and expensive cost in an experimental study [6].
3) Capable in revealing atomic-scale structure evolution [14], and some mechanical properties at macroscopic-level of matters and experiments that can be interpreted at the atomic-scale by means of MD simulation [9].
4) The MD simulation has shown its advantages to track the atomic movement (atomic trajectories) since it treats atom as a classical particle and solving their Newtonian equation of motion [23] and also studying the related diffusion phenomena at nanoscale [14].
5) Computer simulations, which include the MD simulation, is provide full spatial resolution throughout the failure processes, allowing macroscopic stresses to be directly related to the molecular structure and dynamics. Recently developed methods also enable the tracking of entanglements on a microscopic level [45].
6) Of all the powerful numerical models at the nanoscale, molecular dynamic simulation has outstanding advantages; not only provide the steady state of a system, it can also simulate the non-equilibrium process under various conditions, which helps to investigate surface contact and boundary lubrication at the nanoscale [53].

Meanwhile, the disadvantages of MD simulation in the joining process are:

1) Generally, the precision of MD simulation is less than that of the quantum mechanics, but MD has the advantages of generality, less calculation and high efficiency [54].
2) However, the dynamic processes, performing in the CPMD still restricted to a small system which is the main disadvantage of CPMD [55].

4. Conclusion

Molecular dynamics (MD) simulation was introduced to fill the gap between theoretical prediction and experimental results. Molecular dynamics simulation had been shown its advantages to simulate the various joining processes that are diffusion welding, explosive welding, friction stir welding, linear friction welding, cold welding/nanojoining, and thermal bonding with various material in atomic-scale. Experimental study of the joining process is expensive and can be hardly achieved due to the sensitivity of the material at some condition, such as high temperature, high pressure, and rapid growth of melting and crystallization process. Moreover, these condition in the experimental study could lead to lattice mismatch, crystal defects, the presence of impurities, thermal expansion coefficient mismatch and reactions at the interface, which by this method could be avoided. The recent study also has revealed various welded and as-received materials mechanical properties by employing the MD simulation. Even though that some mechanical properties related to the microstructure and the alloys model still have a lack in modelling, the potential use of MD simulation is still looks promising. As the mentioned disadvantages are on the relatively small system and less accuracy due to the use of classical mechanic theory instead of quantum mechanics, this method should focus on these disadvantages, for example by using a larger-scale model and the application of quantum mechanics theory to the MD simulation algorithm. Furthermore, the growth of computer performance has led to the use of large-scale simulation, so that the main focus would be on the implementation of quantum mechanics to its algorithm.

Acknowledgement

The author would like to express his thanks to the management and science university who has funded this project.

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