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A Review of Molecular Dynamics Simulation of Carbon Nanotubes and Nanowires: Joining and Properties

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Abstract: Carbon-nanotubes (CNTs) and Nanowires (NWs), the two nanomaterials with outstanding properties, are the materials with which their behaviour and properties have long been drawing attention to researchers. However, the tiny nature of these two materials causes difficulties in describing and estimating their behaviour and properties, thus a numerical technique that considers the tiny nature of the materials like Molecular Dynamics (MD) simulation is a promising solution to this problem. Since the early utilization of MD simulation in the investigation of the behaviour of carbon-nanotubes and nanowires, it provides the researcher with an excellent description of how the two materials behave at atomic-scale and then estimate their properties. Recently, MD simulation of CNTs and NWs exhibit growth in the simulation size as with the growth of the computing capabilities. The size of the materials being simulated by MD simulation increased significantly in the recent year, thus giving possibility to achieve a better description of the behaviour and a more precise estimation of the properties. In this review, we provide an overview of the recent advances in the investigation of the joining processes and properties of carbon-nanotubes and nanowires at atomic-scale utilizing molecular dynamics simulation.

Keywords: Carbon Nanotubes, Joining, Molecular dynamics, Properties, Nanowires

1. Introduction

Joining of materials is one of the highest demand activity in the industrial sectors [1–3]. The process of joining materials is known taking a lot of costs, either on its research to get the most efficient method and parameters such as pressure, temperature and welding time or in the industrial activity itself in which related to production processes. In terms of research, those cost problems have made some researchers performed their works by using a numerical method, such as molecular dynamics (MD) simulation. Molecular dynamics simulation is a promising method to investigate the behaviour of the material at the atomic-scale since it is not limited by sample preparation and testing condition involved in most experimental work, which is required for most of the joining process [4], therefore the cost of research could be reduced significantly. In some cases, where a classical description of the system is adequate, the continuum method based on finite element might be used. However, such a method is limited to its size and when the case of welding at the nanoscale is required, such as to join Carbon Nanotubes [5] and Nanowires [6], this particular method becomes lacking. Here is where MD simulation comes into play its role [7]. Its ability to deliver a nanoscale investigation of the various materials and behaviours has made MD simulation one of the most used numerical methods in nano-sized materials, such as carbon nanotubes (CNTs) and nanowires (NWs).

The method of classical MD simulation is mainly built upon the solution of the Newtonian equation of motion numerically which runs under a particular ensemble of atoms [7]. Hereafter, a solution of the equation of motion is

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integrated into a very short range of time (about 2-3 femtosecond). To study the atomistic behaviour of a particular material, the classical or semi-classical interatomic potential of a particular atom, namely interatomic potential, must be addressed first. The interatomic potential defines the behaviour of every atom inside a simulation system, for instance, kinetic energy, potential energy, and the changes that may occur due to the applied parameters, such as temperature and pressure. It is critical to choose a proper interatomic potential if one wants to study material at the atomic scale using MD simulation. In fact, in most cases, it defines the quality of the performed simulation. Some potential models have been successfully developed, like Lenard-Jones [8–10], Embedded Atom Method (EAM) [11–13], Tersoff [14], Tight Binding [15], Brenner [16], Finnis-Sinclair [17] and so on. Every interatomic potential model developed is most likely used specifically for a particular material, for instance, EAM many-body potential that has been developed for use in the investigation of metallic materials like Cu, Ag, Au, Ni, Pd, Pt [12]. Finally is the ensembles of atoms. This particular aspect defines the states of the system statistically [18]. It is not only for probing purpose, which will allow one to know the state of the system, such as the temperature and pressure, but rather also related to the controlling issue of which is very critical. The atomic ensembles then allow one to control the parameters within the system into a specific value, therefore study for an extreme condition (very high temperature, pressure, energy beam, and so forth) is possible with MD simulation. The Newtonian equation of motion, interatomic potential model, and atomic ensembles is then integrated by an algorithm to produce the atomistic simulation. It is worth mentioning that there is an opportunity to gain accuracy and precision of the atomistic simulation by considering quantum-based simulation that integrates Hamiltonian-based equation. However, quantum-based simulation known very complex that increasing the number of atoms will lead to an exponential growth of the calculations necessary to finish the simulation [19]. This issue in quantum simulation prevents this method to be adopted in a very large-scale simulation, like a study reported by Shibuta et al. [20]. Other than that, classical MD simulation has tremendous advantages and several well-established algorithms to integrate the Newtonian equation of motion. The algorithm that most likely adopted in MD simulation is based on the Verlet algorithm [21], in which further developed as Velocity Verlet. Another algorithm like the Leap-Frog algorithm is widely used for various application, but since the Verlet algorithm brings many improvements in the computational correctness and speed, the Verlet algorithm has dominated as the most used algorithm in MD simulation. One of the free and open-source software that integrate Verlet algorithm is Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [22].

Nowadays, MD simulation is used by many researchers to investigate the behaviour and properties of various materials, like the deformation behaviour that involves applied temperature and pressure and their mechanical, electrical, and thermal properties. These properties are so important when it comes to the application in industrial processes, thus precise estimation of these properties for a particular material is necessary. Outstanding properties of carbon nanotubes (CNTs) and nanowires (NWs) nowadays bring a lot of attention since its first invention, especially for a candidate of nanomaterial in electronic devices. Furthermore, it has a broad range of application, such as miniaturization of electronic devices logic gates [23–25], solar cells [26], atomic-scale mass sensing [27], and for battery and capacitor [28–30]. The nano-sized materials like CNTs and NWs are then suitable to be investigated with MD simulation because this method is built up for such a scale.

2. Molecular Dynamics Simulation on The Modelling of Joining Carbon-Nanotubes and Nanowires

As the development of carbon nanotubes and nanowires grow rapidly, the investigation of the properties of these materials in an intriguing aspect to be investigated, especially when it is joint with similar or dissimilar materials. The difficulty, for instance, that caused by the ultra-small material size, and expensiveness of investigating the material experimentally, has led to another strategy, which is a simulation. In this section of the paper the efforts on the modelling of joining carbon-nanotubes (CNT) and nanowires (NW), include its method that involved position configuration of the joining process, structure, and size of the material, and also the pressure and temperature performed by using MD simulation will be addressed. Before the welding process using MD simulation is presented, firstly the technique to analyze the structural deformation involved during the welding is presented. This technique has already been done through decades to understand the structural evolution that involves the pre-, on-, and post-process of joining material which employed MD simulation.

2.1 Structural analysis techniques in atomistic simulation

To understand the behaviour and mechanism of material at the atomic scale, especially those which employ MD simulation, there is a broad range of technique to analyze the structure and properties of the atomistic simulation, for instance, the technique that based on the nanoindentation [31–33] that mostly used to calculate the elastic modulus and the hardness of the materials [34], the indentation cracking of brittle thin films on brittle substrates [35]; the fracture toughness, adhesion and mechanical properties of dielectric thin films [36]; the strain hardening and recovery in a bulk metallic glass [37]; the phase transformation of titanium dioxide thin films produced by filtered arc deposition [38]; super-hard materials [39], the structural analysis that based on the different lattice structure, such as for general face-centered cubic (FCC) or even specific only for a particular structure such as body-centered cubic (bcc) [40] and hexagonal close-packed (hcp) materials [41]. These techniques have bring-up the possibility to analyze the phenomena of crystal

defects or even calculate the material properties. For instance, the first structural analysis technique is "common neighbor analysis" (CNA). The basic idea of the CNA technique is decomposing the Radial Distribution Function (RDF) [42] concerning the environment of the pairs. The pairs of atoms are firstly classified by (1) whether or not they are near-neighbors, (2) the number of near-neighbors they have in common, and (3) the near-neighbor relationships among the shared neighbors [43]. This technique has already been developed to obtain more valid and specific data, such as for the characterization of multi-phase systems [44] and to characterize the alteration under crystalline deformation for multiple structural symmetry groups [45].

To study the structure of the plastically deformed thin film in detail, Kelchner et al. [46] have proposed a method that is centrosymmetry parameter (CSP). In their proposed method, the centrosymmetric materials (material with FCC structure) will remain centrosymmetric under homogenous elastic deformation and each atom has pairs of equal and opposite bonds to its nearest neighbors. As the material is distorted, these bonds will change direction and/or length, but they will remain equal and opposite. When a defect is introduced nearby, this equal and opposite relation no longer holds for all the nearest-neighbor pairs. The centrosymmetry parameter for each atom is defined as follows:

$$P = \sum_{i=1,6} |R_i + R_{i+6}|^2 \tag{1}$$

where R_i and R_{i+6} are the vectors or bonds corresponding to the six pairs of the opposite nearest neighbors in the fcc lattice. Another method, that is common neighborhood parameter (CNP) [47] techniques is then proposed by employing the advantages of both CNA which characterizes by using statistics of diagrams formed from a given arbitrary local atomic configuration, and CSP which give a measure of the deviation from the centrosymmetry in the vicinity of a given atom. This technique proposed a new parameter obtained by put together these two methods, Q_i, for each atom i in the structure. The Q_i is defined as follows:

$$Q_i = \frac{1}{n_i} \sum_{j=1}^{n_i} \left| \sum_{k=1}^{n_{ij}} (R_{ik} + R_{jk}) \right|^2 \tag{2}$$

where the index j goes over the n_i nearest neighbors of an atom i, and the index k goes over the n_{ij} common nearest neighbors between atom i and atom j. R_{ik} is the vector connecting atom i to atom k.There are more two other methods developed based on the CNA method, they are dislocation extraction algorithm (DXA) and bcc defect analysis (BDA). DXA is proposed to be a fully automated way to extract the dislocation lines from atomistic simulation data. It is generating a geometric description of a dislocation network that fulfils the Burgers vector conservation rule at each node. Meanwhile, the bcc defect analysis (BDA) [41] method is a method that particularly proposed for analyzing the materials with BCC lattice. The novelty of the BDA method is that not only the atom itself but also each of its neighbors is evaluated against characteristic defect criteria. To this end, all atoms within the cutoff distance are classified according to their values of CN and CSP. However, basal plane vector cluster analysis (BPV-CA) also proposed a specific material structure that is hcp [48] which has a unique basal plane. Since this material deformation is driven by complex mechanisms related to slip-twin interaction, the current dislocation theories are still not clearly explaining for such thing. This method determines the direction of the normal to the basal plane for each atom. Since every twin system and twin variant has a unique miss-orientation from the original structure, the BPV method is capable of uniquely identifying the parent and all variants of twins. The BPV cluster analysis (BPV-CA) assigns each atom to a cluster based on this distinct orientation and that of its nearest neighbors. Meanwhile, the slip vector analysis (SVA) also could be used to analyze the structural defects. The slip vector analysis for the atomistic simulation was firstly proposed by Zimmerman et al. [49] to examine the nanoindentation of Au(111) crystal which both near and far from the surface step. The analysis that based on the nanoindentation could be useful particularly in the process of defects creation, which involved critical energies and stresses, such as in the machining processes [7]. Although there are many more parameters that need to be considered during the process, the slip vector analysis that based on the nanoindentation could be used to both quantify the Burgers vectors and determine the dislocation in the crystal [50]. The slip vector developed by Zimmerman is defined as:

$$s^{\alpha} = -\frac{1}{n_s} \sum_{\beta \neq \alpha}^{n} \left(x^{\alpha\beta} - X^{\alpha\beta} \right) \tag{3}$$

where n is the number of nearest neighbors to atom α, n_s is the number of slipper neighbors, and $x^{\alpha\beta}$ and $X^{\alpha\beta}$ are the vector differences of atom α and β current and reference position, respectively.

Ackland-Jones [40] also had proposed a technique for structural analysis of materials. The post-simulation problem of MD simulation particularly brings up the problem to determine the local coordination, distinguishing fcc, hcp, bcc, and other relatively close-packed structures which in this case could be resolved using a method proposed by Ackland

and Jones. This technique had been used by many researchers. This method is built up based on a heuristic algorithm to define and analyze the local structure of simulated solids and display the results by color coding particles to reveal regions with bcc, fcc, or hcp crystal structure. They have eschewed from "mathematical elegance" and instead, they concentrate on heuristics which can be rapidly implemented using the information readily available in the radial and angular histogram (radial distribution function (RDF) and angular distribution function (ADF)). Thus, the angular distribution function is described by eight numbers (Xi), the number of angles in the region of θ_{jik} chosen to reflect angles present in the most likely phases. Distinctive characteristics of the combination of the X_i^S were then sought which directly measure differences between the possible structures and are persistent even under significant deformation.

2.2 MD simulation on joining CNT and NW

There are a few techniques that have been developed to join CNT and NW. These techniques are necessary to satisfy the shape and technical properties needed for a particular application in nanotechnology. Since CNT and NW in an extremely small regime and involving the very precise technique and apparatus to join them, therefore it is difficult to investigate the behaviour and properties of those materials. To fill the gap MD simulation is introduced, although several limitations yet to be fixed, such as at the estimation of the induced pressure although it is still enough for such simulation. However, a great insightful idea regarding the behaviour of CNTs and NWs at the atomic scale by MD simulation has made this simulation method widely used. In this part of the paper, the joining technique and methods that are reported in the literature at which employing MD simulation is discussed in detail.

2.2.1 Joining CNTs and CNTs

One of the very first efforts of joining CNT is induced by Krasheninnikov et al. [51]. This study theoretically investigates ion-irradiation to forming a nanotube junction. Unfortunately, the result is that the forming of nanotube junction using this method only could be reached at relatively high temperature, that is 2000 K so that the experimental investigation is impossible to be done. In their simulation, they predict that the optimum Ar ion energies needed to provide this welding is in range of 0.4 — 0.6 keV and the irradiation doses are about 1015 cm-2. Meanwhile, using electron beam irradiation, Jang et al. [52] have demonstrated that to perform precise welding as previous work by Krasheninnikov, they need temperature range from 1600 K to 3500 K, but in the experiment, the more steady temperature is about 1000 K with the electron beam energy of 50 keV. A model by Jang et al. could be seen in Figure 1(a).

Another way to join CNT and CNT have performed by Yang et al. [53]. They have reported a novel welding method of single-walled CNTs (SWCNT) at an experimentally relevant temperature which facilitated by nanobuds to create a C-C bonded junction formation between CNT. One of the main problems in joining CNT-CNT is that this joining process requires a relatively high temperature that is > 4000 K which is too high to be applied to experimental work. Therefore, this could be a breakthrough in this process. Figure 1(b) has demonstrated the bonding of CNT-CNT through nanobuds.

The difficulty in the fabrication of CNT and CNT, especially in the axial direction, has been an obstacle to the quality of the connection and practical application of CNT in nano-electronic devices so that the fabrication method should be developed. Cui et al. [54] have investigated the possibility of this challenge by welding the CNT-CNT in the axial direction through the nanoparticles melting. The configuration of nano-welding is mainly dependent on the critical distance and the effective nanoparticles number in the actual experiment. Core filling factors such as the diameter of CNT hydrophily and roughness of the substrate material also have influenced to the nano-welding process, which is necessary to study to obtain high-quality of the solder joint between CNTs in nano-welding process. A comprehensive study on joining CNT-CNT also has performed by Cui et al. [55]. They report a method to join CNT-CNT facilitated by 2 nm Ag particle which has a melting point at 605 K. The terms of soldering that they were used is like the welding itself. Most of the results almost the same. They have demonstrated these processes with different diameter of CNT and at several temperatures. Even though these temperatures are different (600 to 900 K), it will only impact the Ag particle since CNT has a much higher temperature to be deformed. Figure 1(c) shown the study by Cui et al. [53,54].

For some circumstances when joining between CNT is necessary, it is difficult to deal with the strong bonding between the carbon atoms in CNT. MD simulation of joining CNT-CNT has shown to be reasonable in simulation, yet it is hard in a practical point of view. This is due to the fact, other than high temperature and high energy beam, its characterization is pretty much involving complex parameters that must be controlled and therefore further study in both simulation and experiment is inevitable if the technology of CNT wants to be applied in the industry of nanotechnology.

2.2.2 Joining NWs and NWs

Many researchers have performed investigations on how to join the NWs and NWs. One of the very first cold-welding efforts of joining NWs and NWs is research by Lu et al. [6]. These experiments used Au ultrathin nanowires welding in ambient temperature, that is about 300 K. By using high-resolution Transmission Electron Microscope (TEM) and in situ measurements, the welding results are nearly perfect, which mean are with the same crystal orientation, weld strength and the electrical properties of all parts welded NWs is indicating a good welding quality. These high-quality welds are promoted by nanoscale sample dimensions, mechanically assisted fast surface-atom diffusion and oriented-

attachment mechanism. Also, these experiments are demonstrated between Au-Ag, Ag-Ag and indicate that the technique may be generally applicable to all these metallic materials. The investigation of this cold welding, with low stress, no friction, and no heating involved during the process in nano-sized materials would be a great interest to develop new devices. Also, the nano-sized material made NWs characteristics and properties appropriate to be investigated via molecular dynamics simulation.

Besides using the cold-welding method, in which we know that it shows great results, some investigation also reveals the welding process using various conditions and temperatures. These NWs-NWs joining processes research that using the MD simulation method could be divided into three different focuses, which is based on the condition and temperature, based on the structure and size, and based on the position configuration.

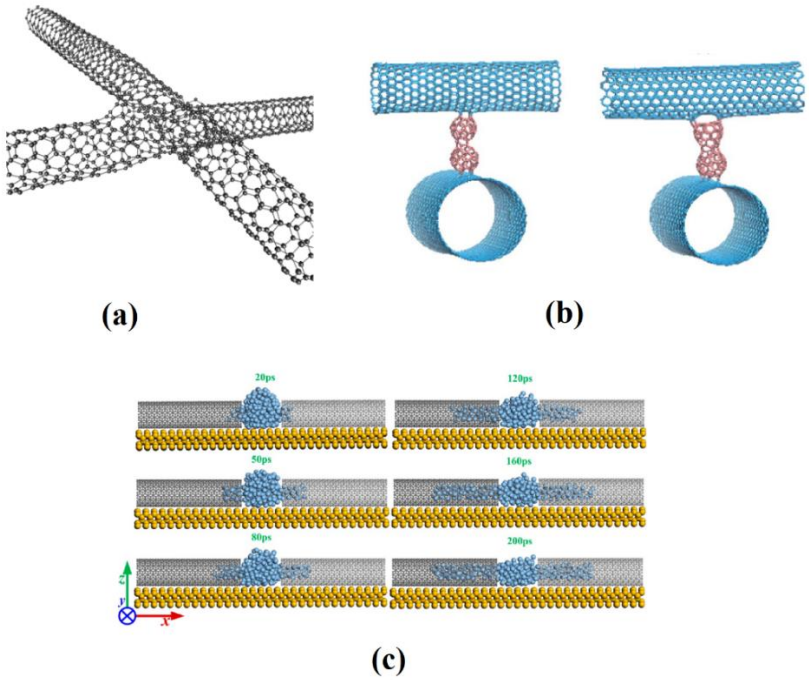

Fig. 1 - (a) Final result of CNT-CNT welding after electron beam irradiation and annealing with a diameter of 7.5 Å and chiral index of (5,5) -(5,5) [52]; (b) final result of CNT-CNT welding with different diameters (±2 nm) and chirality ((18,0)–(30,0) and (10,10)–(26,0), respectively) welded and facilitated by nanobuds at a temperature of 1500 K [53]; and (c) final result of welding CNT-CNT via 2 nm Ag nano-particle with the chirality index of (15,15)−(15,15) [53,54]

MD simulation on joining NWs-NWs in various conditions and temperatures

Wu et al. [56] have investigated the possibility of joining NWs under various temperatures, ranged from 300 K to 900 K. The details of the NWs models of their research are shown in Figure 2(a). They were used not only Au and Ag pair, but also Au-Au, and Ag-Ag pair as research sample. Among the three mentioned pairs, their simulation indicates that the Au-Au NWs pair has the best welding quality, and the Au-Ag pair is the worst one.

An intensive study had been done by Zhou et al. [57] which focus on simulating the cold welding under the various condition, that are: moving rate from (a) 5 m/s (0.05 Å/ps), (b) 10 m/s (0.1 Å/ps), (c) 20 m/s (0.2 Å/ps) (d) 40 m/s (0.4 Å/ps); diameter from 4 nm to 16 nm with an incrementor of 4; temperature is ranged from 150 K to 750 K (150 K, 300 K, 450 K, 600 K, 750 K); crystal orientation is various in [1 0 0], [0 1 0], [0 0 1], and [1 1 0], [0 0 1], [-1 1 0] directions; metals used is Au, Ag, and Cu. A critical issue of this research is coming from its ability to join different metallic NWs and that had been made the breaking behaviour also different. It indicates that the atom displacement taking consideration of breaking the welded NWs when it occurs on the stretching stage. Figure 2(b) is shown the schematic configuration of welding Cu-Cu NWs and a full stage of joining a sample of Cu-Cu NWs. This sample is welded under 10 m/s move rate, meanwhile, the temperature is set to an ambient condition that is 300 K (cold-welding).

Hu et al. [58], also has demonstrated to join NWs by using the diffusion bonding method with Ni and Al materials utilizing MD simulation. In their simulation, they used four different temperatures that are 1 K, 300 K, 500 K, and 700 K. They have found that, by increasing the temperature, the thickness of the interfacial region is also increased, which shown in Figure 2(c).

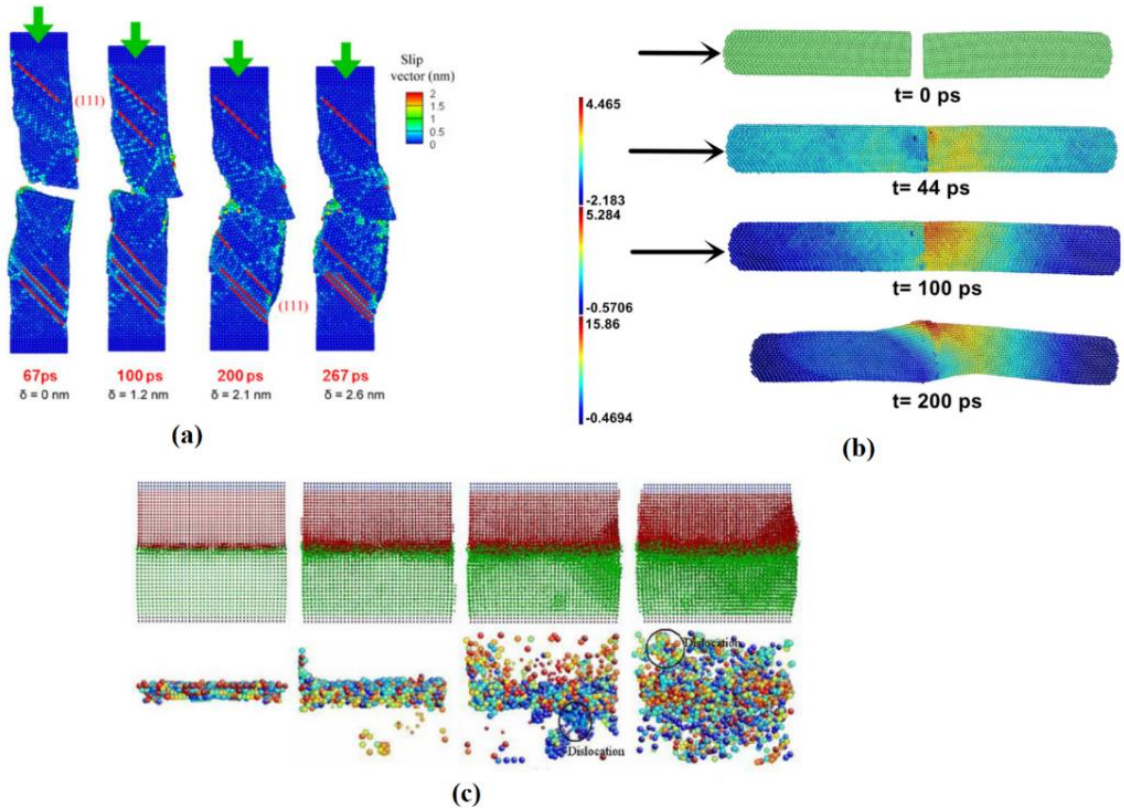

Fig. 2 - Cold-welding of various NWs with different condition and temperature along with its displacement analysis (a) detailed structural change during cold-welding of Au-Ag NWs for different interferences and timesteps [56]; (b) cold-welding of Cu-Cu NWs undergoing cold-welding at the different timesteps [57]; and (c) diffusion-bonding of Al-Ni NWs with different temperature and its corresponding structural differences [58]. The study employs (a) SVA (Slip Vector Analysis); (b) CNA (Common Neighbor Analysis) and (c) CSP (Centrosymmetry Parameters) for their structural analysis

MD simulation on joining NWs-NWs in various structures and sizes

The importance of structure and size of the NWs in joining processes has led to many investigations that try to figure out how much it influences the whole joining parts, such as the weld strength, the deformation of the structure, breaking behaviour and so on. One of the very commonly used metallic materials is the face-centered cubic (FCC) structure, which could be found in the Au, Ag, and Cu materials. On the FCC materials, Huang and Wu [59] have shown that the cold-welding of gold NWs show less variance than with high-temperature, indicates that the cold welding of gold NWs is highly feasible. A similar result also revealed by Wu et al. [60]. The size-dependent of NWs in their simulations indicates that a smaller diameter of NWs will impact the higher welding strength. Figure 3(a) shows the welding strength of each diameter used in Wu et al. simulation.

An intensive study had been conducted by Zhou et al. [61] on the gold composite nanowire. In their simulation, they were used various shape and grain size of NWs. These different samples are based on the structure and size of NWs, also the grain of each sample has a different size which will influence the welding and breaking behaviour. The mechanical properties obtained from the welded NWs are influenced by these structures, size, and grain size differences. The variation of NWs structure and size simulated here could lead to a better decision on determining which is the NWs structure and size would be used that fit to the application needed based on its mechanical properties and breaking behaviour. Even though the chemical and electrical properties of NWs had not investigated here, it was a great idea to conduct NWs investigation based on the structure and size so that another study could follow up later on, especially on the electrical and mechanical properties of various structure and size NWs. To obtain a comprehensive simulation result, Zhou et al. also have conducted to divide the simulation into 2 groups of simulation time. Each group has a different time of welding, holding, and stretching. The difference between the welding and holding time is the influence of the interfacial region thickness, and the difference of stretching time has shown the different of its breaking behaviour. Zhou et al [61] have shown that the different structure and size is important to achieve the desired mechanical properties of a welded NWs.

They employ a different welding phase, and Group II has a longer welding time. It influences to the deformation that promotes joining is demonstrated more by this Group II compared to the Group I. This longer welding phase has shown

that the deformation has created various of changes in the structure of the gold composite NWs. The domination of FCC in the before welded phase structure has less than the after welded phase. Meanwhile, even though the Group I have less deformation than Group II, the Group II simulation has better contact area. There are no significant differences from the stretching phase of the two groups of gold composite nanowire models. Figure 3(b) shows an interesting phenomenon involved in the post-processing of cold-welding gold composite NWs, that is a tensile test. It is observed that bigger NW size has a few correlations to a breaking phase, that it has a narrow breaking phase compared to those with a smaller size. However, when it comes to the grain size, the problem becomes more complex related to the Hall Petch effect [62], which in the study by Zhou et al. not clearly discussed.

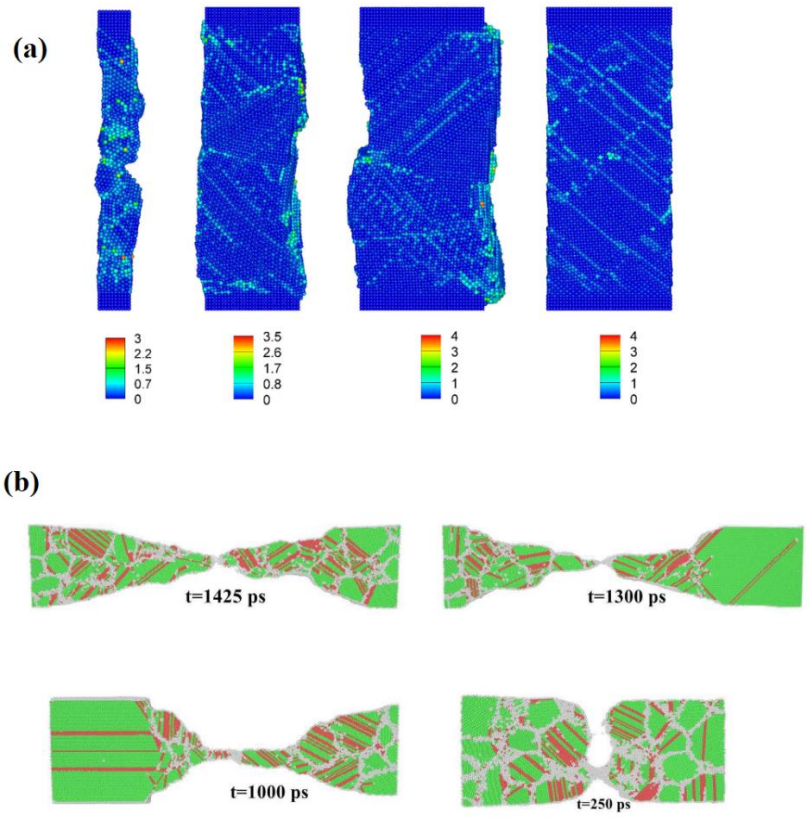

Fig. 3 - (a) Snapshot of cold-welding Au NWs with different size [60] and (b) snapshot of tensile test of Au NWs with different shape, size and grain-size when they are about to break and its corresponding time [61]

MD simulation on joining NWs-NWs in various positions configuration

In the case of joining materials, it is not only focused on joining it by head-to-head configuration. Sometimes, the T junction or Y junction is needed to be formed based on the needs of a particular device. Therefore, some investigation on joining NWs-NWs have done in various position configuration. In this subpart of the paper, the concern is to address those studies.

As demonstrated by Pereira and da Silva [63], which is focused on the cold welding of gold and silver nanowires in the axial position configuration, they have shown the possibility of joining metal NWs via cold welding in this classical configuration. One of the very interesting results of this study is that this metallic NWs could reconstruct their face-centred cubic structure which lost during the cold-welding process that influenced by the plastic deformation and then ends up with the results of very few defects for the final cold-welded NWs. Besides, Cui et al. [64] also do a similar simulation using this position configuration. But, instead of just modelled for the cold-welding method, they also develop a model for some various temperatures to figure out the different behaviour of such configuration. However, they both conclude that the most suitable method for welding nanowires is by employing cold welding, and it is concluded that their work could strengthen to use cold welding method (in temperature of 300 K), instead of diffusion bonding or else (in temperature of more than 300 K).

Another position configuration of cold-welding nanowires demonstrated by some researchers is when the NWs are in the crossed position [65] and T-like junction [66, 67]. These investigations are initiated by the required method for joining material not only on the head-to-head configuration but also crossed and T-like which we could find from the various application of nano-sized NWs materials on electronic devices and many other else applications.

As well as the study on the axial configuration of nanowires by Cui et al. [64], their research on the crossed position configuration [65] later also concludes that high temperature is not the appropriate method to joining NWs. This crossed configuration model also set up in the temperature of cold-welding that is 300 K. Their study has demonstrated that although the contact has been occurred, which promoted by the mixture of each Ag nanowires, there were still interstices between the two junction and Si surfaces. This could be prevented by adjusting the temperature into the needed transformation of the welded nanowires to achieve a better quality of nano-joint, but it is still necessary to consider the deformation of NWs as well, since if the temperature is too high then it will decrease the stability of the NWs joint. The crossed configuration of cold-welding NWs is demonstrated in Figure 4(a).

The T-like junction position configuration of welding NWs was demonstrated to introduce the complexity of joining the nano-sized material in the ambient temperature and above. Even though Ding et al. [66] has demonstrated the T-like junction of welding Au-Ag NWs, they have more intention to investigate the properties of the end-to-end hybrid joint. But, as we could see in Figure 4(b), they have to manage to complete their investigation with Ackland-Jones and centrosymmetry analysis so that the behaviour on its simulation of the joining process has demonstrated. The movement of atoms and the changing of its structure has been presented by their works. Also in the same position configuration, Wu et al. [67] have more intention to explain such phenomena. They have employed the slip vector analysis to explain the mechanism of nano-welding and how the size of NWs influencing to the welded NWs. The specific result obtained is explained as follow: (1) The top NW elongates just before welding due to the interaction of the van der Waals (vdW) attractive force; (2) During welding, the bottom NW gradually reaches critical bend deformation through successive pressure applied from the top one, followed by buckling of the top NW; (3) The structural order of NWs significantly decreases with increasing welding temperature or decreasing NW width; (4) High-temperature welding (700 K or above) causes alignment difficulty or even failure. Their simulation is demonstrated in Figure 4(c).

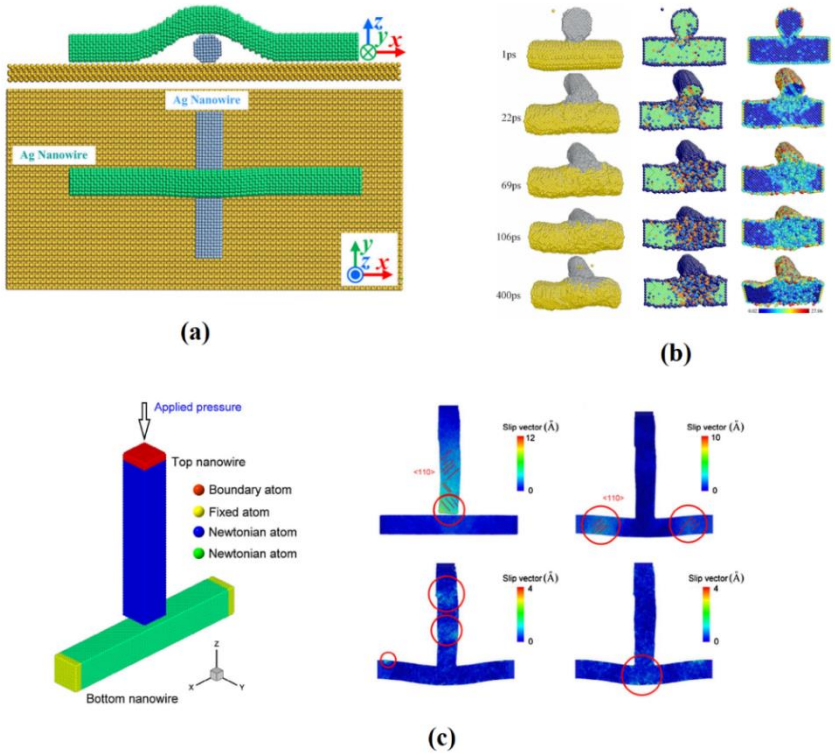

Fig. 3 - (a) Crossed position cold-welding of Ag NWs [65]; (b) Cold-welding of Ag-Au NWs with T-like junction position [66]; and (c) diffusion-bonding (above the room temperature) of Au NWs with T-like junction position [67]

2.2.3 Joining CNT and NW

Nanowires have a potential application on the nanodevices, such as nano-sensors and the other miniaturization of electronic devices. However, NWs are not stable enough that they could not maintain their form for a long time [68], because of the instability of the structure and the sensitivity to the water vapour and oxygen [69], so that the great strength and stability of CNT [70] is promising to be combined to NWs. Employing MD simulation, investigation on the process of joining CNT and NW which means of core filling process has been used by some material, such as aluminium (Al) [71], germanium (Ge) [69], silicon (Si) [72], and silver (Ag) [73,74]. Carbon nanotubes endohedrally decorated with gold (Au) nanowires [75] also shown an interesting phenomenon, even though the tensile properties are not increased with

this technique since gold NWs has a lower tensile strength. Figure 5 shows several examples of the CNT core-filled with Al NWs, Ag NWs, and Ge NWs. The increase of the temperature will lead to the deformation of NWs which leads to the extending of the core-filled area. This concludes that, at a certain temperature, we could control the behaviour of joining the CNT and NWs and get the desired welding result to be applied in the nano-sized materials of nanodevices.

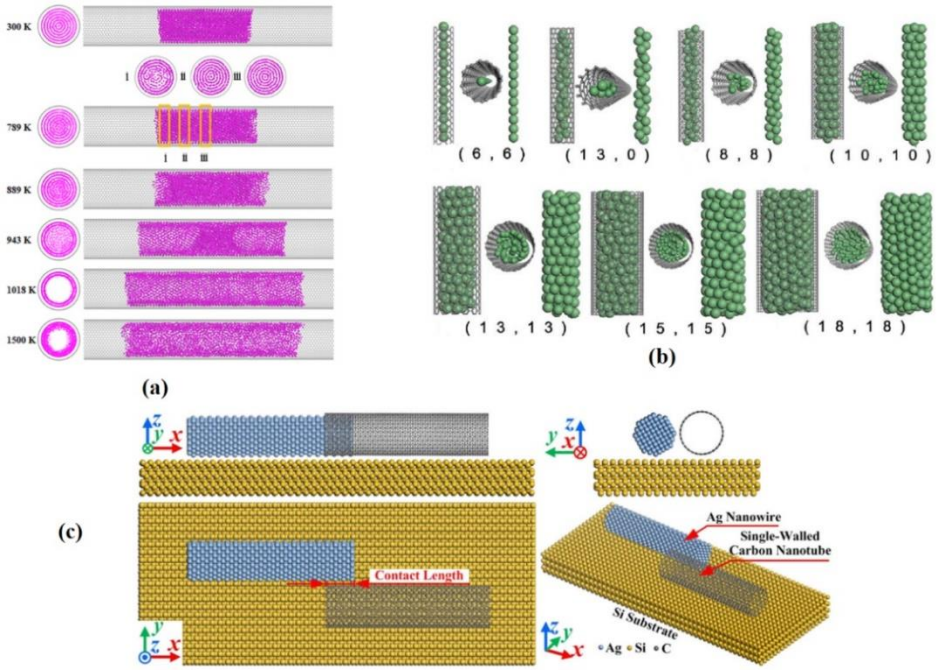

Fig. 5 - Core-filled CNT with (a) Aluminum NWs [71]; (b) Germanium NWs [69]; and (c) Silver NWs [74].

Contact behaviour between two adjacent materials is an important phenomenon in nanotechnology, since it in some sense could exhibit different behaviour compared to the macroscale. In a more detailed study, the contact behaviour of CNTs and NWs that is very critical in building a good bonding quality and structure is addressed by Cui et al. [76,77]. The important of van der Waals energy around the surface of CNTs and NWs reveal its dominant mechanisms in the collapse of CNTs, whilst the energy threshold of the corresponding material has occurred to be consistently maintained regardless the temperature, size effect and other factors. The vdW energy evolution for both aligned and misaligned shaped structure between single-walled carbon nanotubes and metal NWs have shown in Figure 6.

2.2.4 Other Application

Besides the functionalization discussed above, MD simulation also used to investigate the phenomenon of patterning via cold-welding. In this process, a stamp is contacted into the substrates a very thin metal layer has been deposited via cold welding [77,78]. The stamp then separated from the substrate by the subtractive process and material adhere to the stamp, leaving a patterned substrate. Using MD simulation, Song and Slorovitz [80] have demonstrated this process. They have concluded that the film elastically de-bonds from the substrate. This phenomenon occurred before the onset of plastic deformation inside the film during the stamp retraction. Also, the maximum length of elastic de-bond of the film by this simulation has shown to provide a good measure of the degree of damage induced during the patterning process. This process is shown in Figure 7.

Carbon nanotubes also could be welded onto the metallic substrate, as demonstrated by Song et al. [81] utilizing MD simulation which focuses on investigating the relation between surface melting and contact area length. The application of this type of joining material is that carbon nanotubes, in some nano-electronic device, needs to be welded onto metal electrodes which can induce high power consumption at the contact. They have found that there is a close relationship between the melting of the metallic surface and contact area length. Also, the wetting property has a great impact during welding. Therefore, the contact length is dependent on the surface melting propagating and the type of metal should be selected properly to get the proper wetting property. This process is demonstrated in Figure 8(a). Meanwhile, specific nano-welding from CNT onto Ni substrate has been demonstrated by Liu et al. [82]. They have shown that the nano-welding of CNT and the Ni substrate could be accomplished at a temperature of 1500 K which is below the melting point of Ni (1726 K). Also, nano-welding is influenced by the high-frequency ultrasonic energy that softening the Ni metal and causing the plastic deformation under the clamping stress. This process could be shown in Figure 8(b).

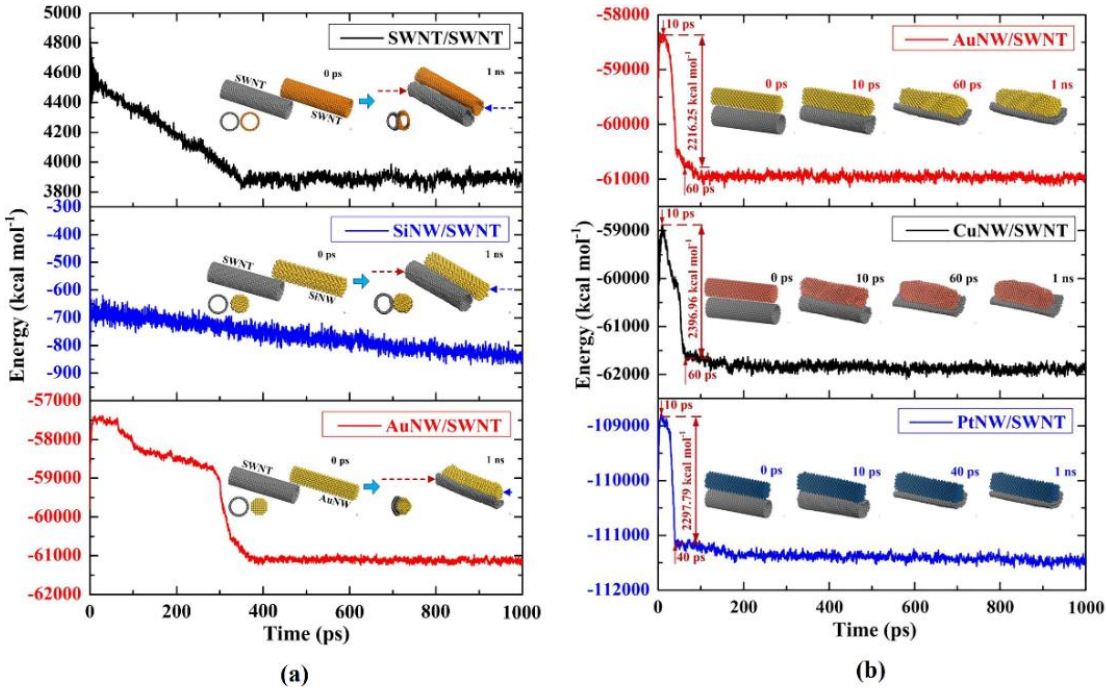

Fig. 6 - The vdW energy evolution of (a) misaligned and (b) aligned side to side shaped structure between single-walled CNTs and metal NWs at 500 K [76,77]

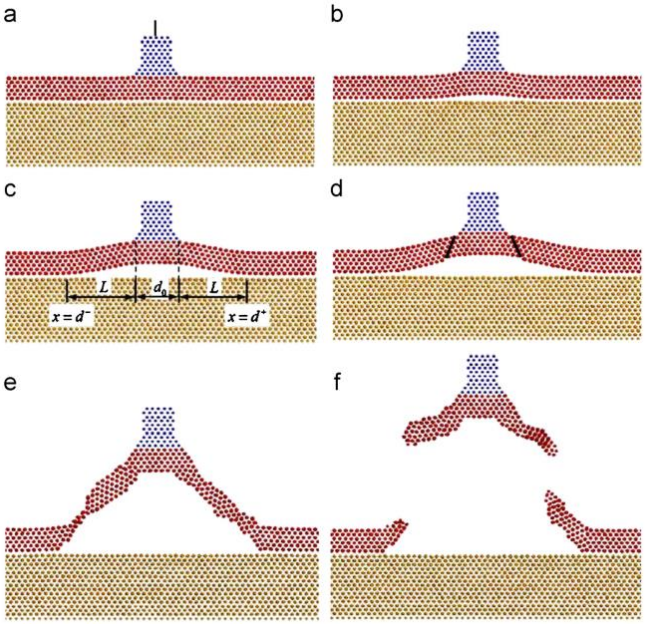

Fig. 7 - The atomistic view of the system in [1 1 0] direction: (a) initial configuration; (b) the thin film elastically starts to de-bond; (c) the de-bond length of the film reaches its maximum; (d) onset of plasticity inside the film;(e) further retraction of the stamp away from the substrate; (f) failure occurs in the film and a section of the film is transferred to the stamp [80]

Another intensive study has been reported by Nian et al. [83] on joining silver NWs onto a flexible substrate. They were used pulsed laser irradiation (Laser Induced Plasmonic Welding) under controlled conditions. This process has shown generate local crystalline nano-joining of silver NWs without affecting regions near the network, which results in a significantly improved optoelectronic performance. The MD simulation of this process has shown in Figure 9.

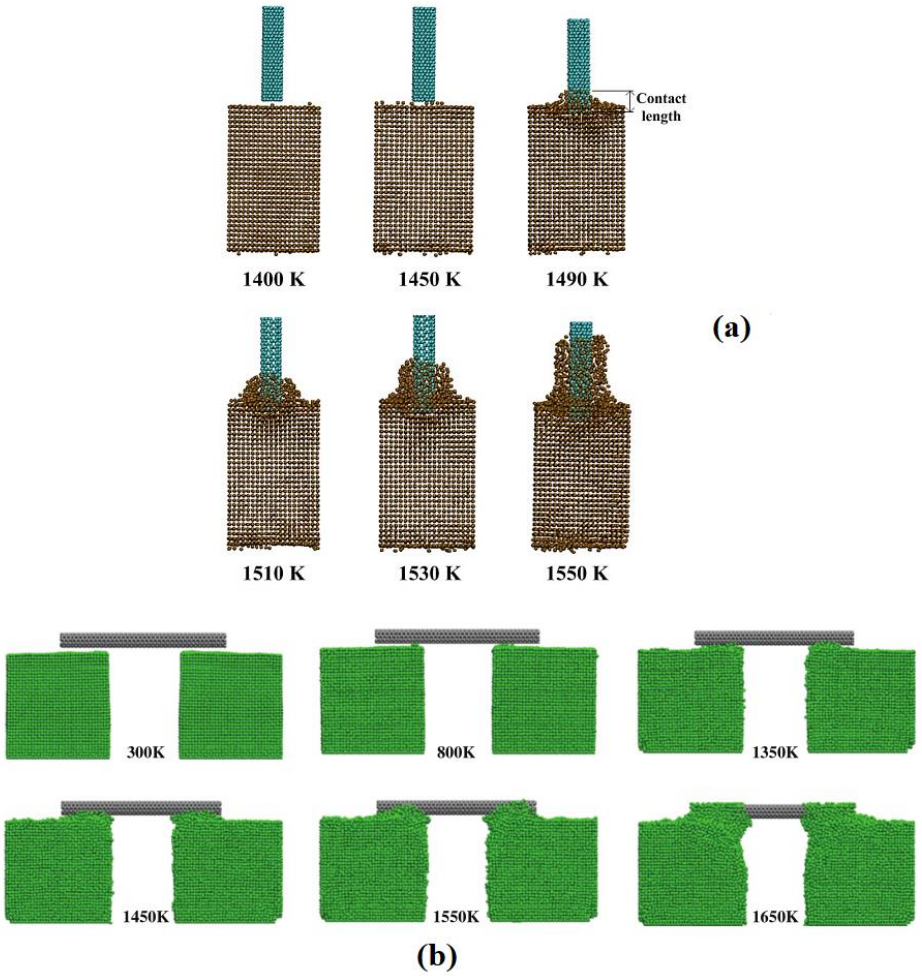

Fig. 8 - Welding of CNT onto Ni substrate with different configuration (a) vertical [81] and (b) horizontal [82]

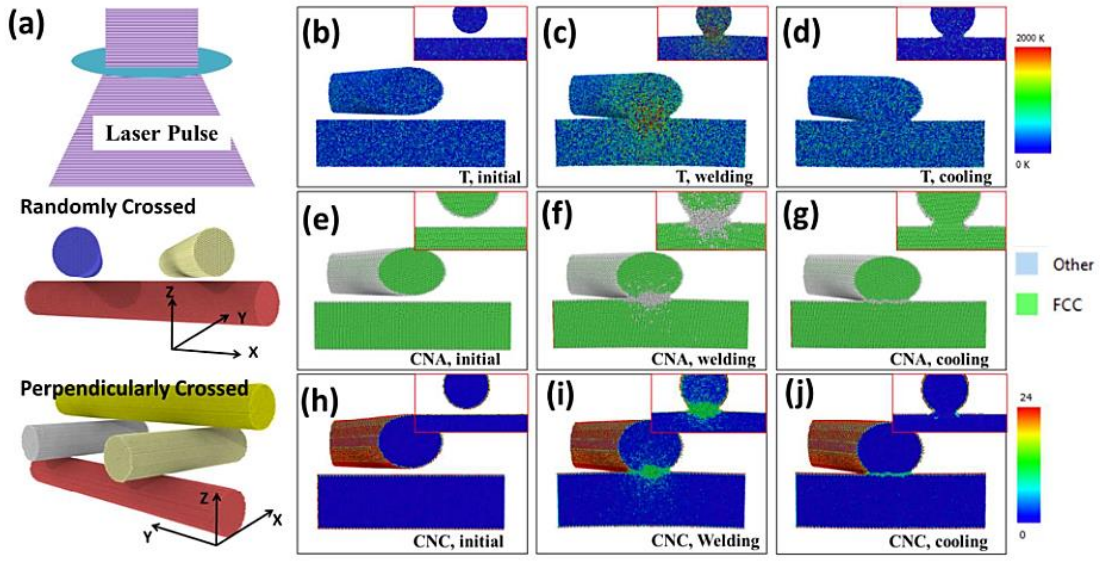

Fig. 9 - MD simulation of nano-joining of Ag NWs onto a flexible substrate using Laser-Induced Plasmonic Welding (LPW). (a) simulation setup; temperature evolution during (b) initial condition, (c) welding and (d) cooling. Structural evolution of FCC Ag NWs during (e) initial condition, (f) welding and (g) cooling. Nanowire ordering structural evolution during (h) initial condition; (i) welding and (j) cooling [83]

As a summary of the technique mentioned in this section, Table 1 shown the performed MD simulation in joining CNT and NW.

Table 1 - Summary of MD simulation in the joining processes of CNTs and NWs and its employed materials, interatomic potentials, and structural analysis techniques and its corresponding results

Materials	Interatomic Potential	Structural analysis	Obtained	References
CNTs and CNTs	Brenner II	-	Feasibility of welding	[51]
CNTs and CNTs	REBO	-	Feasibility of welding	[52]
CNTs and CNTs through 2 nm Ag NP	COMPASS	-	Feasibility of welding	[53,54]
CNTs and CNTs through nanobuds	AIREBO	-	Feasibility of welding	[53]
Au-Au, Ag-Ag, and Au-Ag NWs	Many-body Tight Binding	SVA	Feasibility of welding, the ratio of welding strength	[56]
Ni-Al NWs	EAM	CSP	Feasibility of welding, tensile behaviour, breaking behaviour, Young's modulus, yielding stress, the flow stress	[58]
Au, Ag, Cu NWs	EAM	CNA	Feasibility of welding, yield strength, mechanical strength, weld-strength	[57]
Au, Ag, Cu NWs	EAM	SVA	Feasibility of welding, weld-strength, yield strength, breaking behaviour, tensile behaviour	[59]
Au-Au NWs	Many-body Tight Binding	SVA	Feasibility of welding, tensile behaviour, breaking behaviour, weld-strength, yield strength, elongation ability	[60]
Au composite NWs	EAM	CNA	Feasibility of welding, breaking behaviour, tensile behaviour	[61]
Au and Ag NWs	EAM	CSP, Ackland-Jones	Feasibility of welding, tensile behaviour, breaking behaviour	[63]
Ag NWs	COMPASS	-	Feasibility of welding in axially and crossed	[64,65]
Ag, Au NWs	Many-body Tight Binding	CSP, Ackland-Jones, SVA	Feasibility of welding in T-like junction configuration	[66,67]
Al, Ag, Ge, Si NWs @ CNTs	COMPASS, AIREBO, force field	-	Feasibility of core-filling NWs@CNTs, electrical transport (V-I response), melting behaviour	[69,71–74]
Cold-welded Au	EAM	-	Patterning via cold-welding	[80]
CNTs-Ni substrate	AIREBO	-	Feasibility of welding, contact configuration	[80,81, 83,84]
Ag NWs-flexible substrate	EAM	CNA	Feasibility of welding,	[83]

3. Estimation of Mechanical, Electrical, and Thermal Properties/Parameters of CNTs and NWs

The properties, either mechanical, electrical, or thermal properties, that involved during the process of nano-welding of CNTs and NWs is as important as joining process itself. Those properties of the as-received and the as-welded material, including the properties of materials after heat treatment, if necessary, is inseparable from the joining processes. Beside the in-situ method to investigate the properties of the nanomaterial that can be performed experimentally [6], MD simulation has shown its ability in the investigation of these properties. Some researchers have indicates that the data obtained by the MD simulation also have shown good agreement with the experimental works [82,83,94,95,86–93]. Therefore, using MD simulation to investigate those properties is reasonable, either in its good agreement or to reduce the cost of research, and also there are broad ranges of techniques to make sure that the MD simulation performed is could be validated [96] to maintain its correctness.

Several properties of CNTs and NWs nowadays could be obtained, including yield strength, yield strain, welding strength, shear strength, melting behaviour, breaking behaviour, Young's modulus. The nanoindentation, which has been extensively investigated [32] is one of the phenomena that further could be as its basis in estimation some mechanical properties, for instance, elastic modulus, Young's modulus, and so on. In this part of the paper, the estimation method of` the mechanical properties of CNTs and NWs is presented. Hereafter, the specific above-mentioned mechanical properties and the validation of the related experimental investigation is presented as a comparison in a table.

3.1 Breaking Behavior

The method that has been employed in the investigation of breaking behaviour of CNTs and NWs is mostly by applying stretching process [96,97] and controlled displacement or strain [99]. During the stretching process, the strength of the sample materials will show its ability to maintain their structure. Once they are break, a critical parameter that involved just before the breaking is then could be shown as a function of time. Several types of research have given attention to these phenomena, especially with regards to the material of CNTs or NWs. These two materials, before and after welded materials, have different properties depending on the size of the material and the parameters applied during the welding process itself, such as welding temperature, pressure, and welding time. The stretching rate or more famously strain rate also has shown its impact on the tested material. Figure 10(a) shown examples of breaking behavior of CNTs and NWs. An extensive study by S. Ajori et al., [100] has been conducted to investigate how metallic glass nanowires reinforced by carbon nanotubes, showing the potential of the strength of carbon nanotubes to reinforce the properties. Such reinforcement is potential to be used in various application, such as in the structural design of a bridge, for instance in the form of carbon fibre [101]. However, the related strength was also connected to the stiffness, thus it will make decrease the ductility that is important for various application, like those in reinforcing the Ni composite [102].

3.2 Elasticity/buckling behaviour/Young's modulus

In the crystal structure materials, either it is fcc, bcc, or hcp like NWs, the method that most likely to be used to quantify and calculate the mechanical properties that related to the elasticity behaviour, such as elastic modulus and young modulus is the nanoindentation phenomena [31–33,35,103]. To perform a calculation and quantification of such mechanical properties in MD simulation, some methods could be used, such as by applying the compressive load which is imposing a gradual axial displacement at constant velocity [103–105]. Even though that buckling behaviour of CNTs can easily occur during the compressive load, the interatomic potential could cause a little bit different results, so that Alian et al. [107], for instance, have employed consistent valence force field (CVFF) when they were investigating the elastic properties of CNTs that have proven success to predict the elastic properties of CNT. Figure 10(b) has shown the example of buckled CNTs and its parameters.

3.3 Fundamental frequency/vibration

Natural or resonance frequency is the frequency of a vibrating system at which the resonance phenomenon happens and the system tends to oscillate at greater altitude and this quality that depends on the geometry of the system as well as its mass and applied boundary conditions is mostly evaluated to investigate the vibrational behaviour of a system [108]. The application of frequency and vibration parameter not only limited to the resonator of electronic devices [109], instead, the mass sensing that expected to be used at the zeptogram level [26,109–111] has shown intriguing attention to researchers nowadays. To the present study, the mass sensing sensitivity that exploiting the vibrational behaviour of the CNT known to be increasing as the size of the CNTs is smaller [113]. Thus, the fundamental frequency is an impressing parameter that will create a breakthrough for the nano-sized material. Figure 10(c) shows the example method of CNTs as mass sensing that exploiting its fundamental frequency behaviour.

3.4 Electrical responses

The electrical response of NWs has been widely investigated. For instance, it is known that the cold-welded Au NWs electrical response has no difference with the not-welded Au NWs [6]. It is interesting to address here that, the electrical response of NWs and CNTs is an intriguing parameter that nowadays could be used as a high-transfer current rate of electrode battery [114], diodes and transistors with p-n junction [114–116], and sensors [118]. The fast charging technology, for example, is expected to use this kind of materials since the high rate capability of current transfer is demanded nowadays. The core-filling NWs@CNTs is already addressed in section 2.3 and for further example. The example of V-I responses of NWs@CNTs is shown in Figure 10(d).

3.5 Thermal behaviour and conductivity

Applying controlled temperature in MD simulation have shown successful results. In either canonical or micro-canonical ensemble, the applied temperature will show its effect on the built system which similar to the experimental works, such as when the system is joined or for investigating the melting behaviour. The critical temperature that involved in the material when it is joined or deformed, especially in the CNTs and NWs, has led to the extensive investigation which not only focuses on the behaviour of the material which depends to the temperature but also its ability to transfer the applied temperature to another different separated material. But, rather than to investigate the thermal conductivity, the thermal behaviour of the sample itself, for example, CNTs is also important, which have an intriguing behaviour that it could still stable at very high temperature (1400°C) [121] which different to typical NWs that at the temperature of 800 K deformation will occur [64] which led to the proposed NWs joining at ambient temperature [6]. Thus, these thermal behaviour and conductivity are important to be addressed because such behaviour will be critical when the material is

used in, for instance, nanodevices. In terms of CNTs core-filled with NWs [122], the heat conduction is also an important aspect, since as in the previous discussion in section 2.2.3, the core filled material may lead to a betterment of the properties, including in the thermal behaviour and conductivity properties.

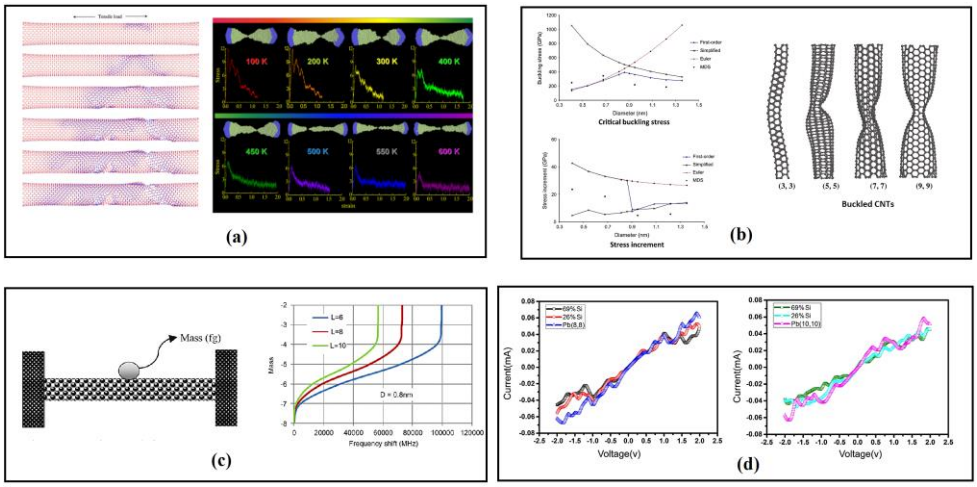

Fig. 10 - (a) Breaking behaviour of armchair CNTs [99] and NWs at the different temperatures [97]; (b) The example of buckled CNTs and its parameter correspond to critical buckling stress and stress increment [119]; (c) the functionalization of the fundamental frequency in CNTs with a schematic of mass sensing and CNTs as a bridge and the response of fundamental frequency in different attached masses and CNTs length (nm) with a diameter of 0.8nm [113]; and (d) the example of V-I responses of Pb-Si NWs inside CNTs with a different composition by employing MD simulation [120]

3.6 Mechanical strength and weld strength

Perhaps, one of the most important mechanical properties of the material is their strength. Their strength, either welded or not-welded material, is important to be addressed because of the relation between the ability to remain their structure in ambient temperature and its functionalization. Even though the welding process will reduce the mechanical strength, welding of NWs in ambient temperature, for instance, has shown very good results [6]. Also, the strength of NWs has shown its dependent on its size [123]. In an experimental investigation, these mechanical properties could be obtained by using the in-situ method. However, MD simulation has shown its ability to measure the mechanical properties of CNTs and NWs by applying a tensile load to figure out the stress-strain relation, or even calculate it by employing continuum mechanics theory or molecular mechanics method [124]. Recently, the mechanical behaviour of MoS nanowires has been reported by employing MD simulation [125], showing the opportunity to use MD simulation to study the broader mechanical behaviour for various materials.

4. Discussions

4.1 MD simulation in general

Performing an MD simulation of welding various materials is known to bring many benefits, such as decrease the development cost, no need to do a sample preparation, and a relatively short time to find the best parameters that fit the relatable problem in joining processes, especially those that work in the nano-scale region [3]. However, MD simulation must be performed precisely correct for figuring out the real phenomena. Interatomic potential parameter, for example, that being one of the factors that have a huge impact on the simulation results, should be chosen carefully. Some tuning to the interatomic potential model might be needed to accomplish a better simulation result, in case that the simulation runs a complex system. The choice of the timestep, either in femtosecond scale, picosecond scale, or nanoscale, and so the atomic ensemble adopted in the simulation also determine the quality of the atomic simulation. All the factors should be considered so that the simulation is correctly describe the nature of the materials itself. Furthermore, the complexity of MD simulation that has so many applications, such as in physics, chemistry, biology, and material engineering had made MD simulation not standardized properly. There are long journeys to gain the benefits and usefulness of MD simulation in science.

Despite the benefits gained by MD simulation, determining a good estimation of parameters in the joining process for a larger material is hard to achieve. This is due to the dependent of size in MD simulation, makes it exponentially more complex when the size of the system that is going to be simulated increased. As a result, customization of the system by a trivial adjustment is necessary based on the experimental work. Nevertheless, the chances of classical MD simulation come when the study of material focused on revealing the dominant mechanisms of a phenomenon, such that

in diffusion welding [158]. The parameters resulted from diffusion welding, like temperature, pressure, welding time and output parameters like stress-strain relation during the tensile test of a diffusion-welded material becomes quite hard to verify. Moreover, materials that can be simulated in MD simulation is a bit limited, because the interatomic potential of the complex materials with a lot of alloying elements like stainless steel and composite is very hard to build, whilst nowadays materials is mostly a complex material with many alloying elements and rarely of the are pure/simple material. It is then hard to find a material that both can be simulated in MD simulation and has the experimental work counterpart. Therefore, focused on the phenomena like diffusion and atomic exchange between two materials in diffusion welding and its related processes are a strong point of MD simulation, because the atomistic view of it might give us an insight for tuning it with specific behaviour and then finally improve the properties.

Summary of the investigation on mechanical, electrical, and thermal properties of welded and not-welded CNTs and NWs Obtained by employing MD simulation and its validation with experimental investigation.

Table 2 - Summary of the investigation on mechanical, electrical, and thermal properties of welded and not-welded CNTs and NWs obtained by employing MD simulation

Research focus	Material(s)	Mechanical/electrical/ thermal properties/ parameters obtained	Additional Information	Reference(s)
Mechanical properties of CNT under various condition	CNTs	Stress-strain, Young's modulus, buckling behaviour, Young's and shear modulus, tensile behaviour	Not-welded	[98,104, 131–134,105,106, 125–130]
Mechanical properties of CNT and graphene with defects	CNT & Graphene with stone-wales defect	Tensile behaviour, strength, Young's modulus	Not-welded	[123,135]
Buckling behaviour of CNT at the various condition	CNTs	Buckling behaviour	Not-welded	[103,118,136]
Mechanical Properties of monocrystalline NWs	Monocrystalline NWs	Tensile behaviour (stress-strain)	Not-welded	[96,97,122,137]
Mechanical properties polycrystalline NWs	Polycrystalline NWs	Young's modulus, stress-strain, breaking behaviour	Not-welded	[138–140]
Fundamental frequency of various sizes and types of CNTs	CNTs	Fundamental frequency	Not-welded	[26,107–112, 141–143]
Electric transport of NWs@CNTs	NWs@CNTs	V-I response	Not-welded	[69,119]
Melting behaviour of AlNWs@CNTs (core-filled)	Al-NWs@CNTs	Melting behaviour	Not-welded	[71]
Joining and mechanical properties of various NWs	NWs	Tensile behaviour (stress-strain), Young's modulus, yielding stress, flow stress.	Welded	[57,58,146, 147,59–61, 63, 66,67,144, 145]
Tensile behaviour of welded CNTs	CNTs	Tensile behaviour (stress-strain)	Welded	[52,148]
CNT reinforcing metals	CNT and metallic materials	Tensile behaviour (stress-strain)	Not-welded	[149,150]
Thermal behaviour and properties of CNTs	CNTs	Thermal behaviour and properties	Not-welded	[151–154]
Thermal behaviour and properties of NWs	NWs	Thermal behaviour and properties	Not-welded	[155,156]
Dependence of temperature, chirality type, and size.	NWs@CNTs	Heat conduction	Core-filled	[122]

4.2 CNT and CNT direct welding

Welding of CNT and CNT directly, obviously, still lacking in the experimental side. All of the efforts addressed here that show the possibility of joining CNT-CNT directly which performed by using MD simulation, however, only could be produced in very high temperature and very high energy beam which is very hard to be accomplished experimentally. Also, the very high temperature ranged from 1500-3500 K as and very high energy beam ranged from 0.4-50 keV [51], [52] that subjected to promote welding of CNT and CNT directly is not considered to be adopted because of huge defects occurred during the process and that it is so complex when it comes to the experimental work. To this matter, the welding parameters that impacted the CNT itself should be addressed first. Furthermore, the outstanding strength of CNT that most probably lost during the welding, if performed, might be one of the most reasonable explanations that had made why welding of CNT and CNT directly is avoided.

4.3 Atomistic investigation trends on the investigation of the properties of CNTs and NWs

Even though the feasibility of welding NWs, either performed by MD simulation or experimentally, is greatly achieved, there are still problems. For instance, for the same materials, researchers tend to use different interatomic potential. For this matter, the validation of the simulation still should be addressed as well in term of the atomic behaviour

and its properties such as mechanical, electrical, and thermal properties. There is a different trend in MD investigation in these two kinds of materials. As MD investigation of NWs mostly focuses on the atomistic behaviour, unfortunately, in some paper it does not address the properties of the materials, such as mechanical, electrical and thermal properties [56,57,146,159]. Acquiring and estimating the properties of a material in MD simulation becomes tricky as the size of the system bigger, especially when it comes for complex material. Even if possible, the results are not good enough to meet the experimental validation.

Meanwhile, MD investigation of CNTs has shown bring many new inventions that exploit the characteristic of it, such as vibrational behaviour (fundamental frequency) that related to the atomic-scale mass sensing application [26,109–111, 160], thermal conductivity and thermal expansion [156,161–163], buckling and structural (for armchair and zig-zag chirality) behaviour including its behaviour when it defected [131,132,136,164,165]. Most properties that accomplished in nanowires material like mechanical, electrical, and thermal properties are also well accomplished and well-addressed in CNTs investigation as discussed extensively in this study. At the first place, the invention of CNTs [5] was bringing many interesting attentions that it comes with an outstanding property compared to the NW, so that the utilization of the properties of CNTs is greatly expected.

4.4 Structural analysis

Some structural analysis methods that have been well-established to perform an analysis of the material defect is merely subjected to be used only for the materials that have some metallic structure, such as fcc, bcc, and hcp. In this matter, investigation of the behaviour of NWs for the various condition which causes defect could be easier, since some methods come with specific software so that it could be used instantly, such as OVITO (Open Visualization Tools) software [166] that comes with some built-in function like common neighbours analysis, vector analysis, atomic displacement, and so on. Different to the CNTs investigation which tends to use an in-house method. Structural analysis of CNTs mostly performed by analyzing the material as it visually looks like. Its structural analysis is also, sometimes, lead to the investigation of its properties, by means that CNTs with armchair structure will have different properties with the CNTs with zig-zag structure, and CNTs with single-walled structure, indeed, will have different properties with double-walled.

4.5 Conclusions

There are a few aspects that are important in joining carbon nanotubes and nanowires. First, the strong bonding between carbon atoms in carbon nanotubes has shown to make it very hard to be joined, unless by using both a very high level of temperature and energy beam/ion irradiation. However, to exploit excellent properties of carbon nanotubes, several types of research have shown that it is feasible to join carbon nanotubes with several metals and semiconductor substrates, shed light on the opportunity to build nanotechnology by carbon nanotubes, such as reported experimentally and fabricated by Hills et al. [167]. Meanwhile, for nanowires, since 2010, Lu et al. [6] have shown that it is feasible to experimentally join nanowires. However, molecular dynamics simulation has gained important insight into the properties of both carbon nanotubes and nanowires, noting several important parameters to join both CNT and NW without losing its impressing properties, either electrical, mechanical, and thermal properties. Also, several atomistic structural analysis tools developed have seemed to gain our understanding of how the structure may be changed during welding, thus prevention can be performed to keep their properties. There are many more opportunities to shed light on an insightful idea of what is going on in the atomic regime by using molecular dynamics simulation. This study has shown that it may be helpful for some degree to use MD simulation, but careless in build the model may lead to sort of miss estimation and interpretation. By carefully selecting and adopting the important parameter to build a model for the nanotechnology system by MD simulation, the usefulness of this method is expected will be gained far better.

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