UDK 620.1:620.168:536.912:01
Original scientific article/Izvirni znanstveni članek

ISSN 1580-2949
MTAEC9, 53(3)367(2019)

APPLICATION OF A MOLECULAR DYNAMICS SIMULATION AND AN AB-INITIO CALCULATION IN COMPOSITE MATERIAL R&D: A LITERATURE ANALYSIS

UPORABA SIMULACIJ MOLEKULARNE DINAMIKE IN AB INITIO IZRAČUNOV V RAZVOJU IN RAZISKAVAH KOMPOZITNIH MATERIALOV: ANALIZA LITERATURE

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Prejem rokopisa - received: 2018-09-19; sprejem za objavo - accepted for publication: 2018-12-17

doi:10.17222/mit.2018.204

Characterising a composite using a molecular dynamics (MD) simulation and an ab-initio calculation is promising in terms of efficiently and accurately uncovering the complicated mechanism of the coupling and interface of the dissimilar materials therein. This paper provides a systematic analysis of existing studies regarding the application of a MD simulation and an ab-initio calculation in composite material R&D. Related literature has been searched, coded, and categorised to capture the distribution and evolution of 22 research topics. Moreover, this study also highlights some of the MD simulation and ab-initio calculation studies, and concludes with a status-quo summary and next round research hotspot prediction.

Keywords: composite, molecular dynamics simulation, ab-initio calculation, literature analysis

Karakterizacija kompozita z uporabo simulacij na osnovi molekularne dinamike (MD) in ab-initio izračun sta s stališča učinkovitosti in natančnosti obetajoča postopka pri odkrivanju kompliciranih mehanizmov združevanja in sobivanja po lastnostih med seboj različnih materialov. Avtor podaja sistematično analizo obstoječih študij, ki se nanašajo na uporabo MD simulacij in ab-initio izračunov v raziskavah in razvoju (R&D) kompozitnih materialov. Tovrstno literaturo je raziskal, kodiral in kategoriziral, da bi zajel in razvil 22 različnih raziskovalnih tem. Nadalje osvetljuje nekaj študij MD simulacij in ab-initio izračunov, zaključuje pa s povzetkom obstoječega stanja ter napoveduje najbolj aktualne teme prihodnjih raziskav.

Ključne besede: kompozit, molekularna dinamika, simulacija, ab-initio izračun, analiza literature

1 INTRODUCTION

Composites are not only the combination of different materials, but also the synergy of excellent performances. The undoubted advantages of composites over other single-component materials push composites forward under the spotlight of both industry and academia. However, composite studies are not easy, owing to the complicated mechanism of the coupling and interface of the dissimilar materials therein, as well as the large number of the potential pairings of constituents.

One efficient way of quantifying the phenomenon and probing the mechanism of composites is by leveraging a molecular dynamics (MD) simulation and/or an ab-initio calculation. A molecular dynamics simulation treats atoms as particles and studies their motion and interactions through the molecular force field,[1] which is calibrated using experimental observations.[2] An ab-initio calculation refers to applying density function theory to forecast interatomic behaviours,[3] which originates from quantum mechanics and involves some simplification to allow an efficient numerical computation.[4] The bottom-up philosophy embedded in these methods ensures the accuracy of the prediction results.

Although a MD simulation and an ab-initio calculation have become common practices in composite material R&D, there has not been a systematic literature analysis that summarises what has been achieved and what to expect. Yet such an analytical study is extremely meaningful in that it consolidates the currently scattered, isolated, and perhaps inconsistent researches, and traces the evolution of the topic's popularity over time.

Based on the above background, this study aims at systematically analysing existing studies regarding the application of a MD simulation and an ab-initio calculation in composite material R&D. More specifically, it unfolds as follows. The method and scope section describes in detail the literature searching and coding process. The literature statistics section reports the categorised research topics and their trend of evolution. The next two sections highlight some of the MD simulation and ab-initio calculation studies. The final section concludes the review with a status-quo summary and next round research hotspot prediction.

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2 METHOD AND SCOPE

2.1. Literature source and searching

The investigated literature in this study was retrieved from either the China National Knowledge Infrastructure (CNKI, a Chinese academic database)[5] or the Web of Science.[6] The search terms include "composite", "molecular dynamics simulation", "ab initio", "first principle", DFT, and their Chinese counterparts. From the search results, the title, year, and abstract of each paper were recorded for further screening.

2.2. Literature screening and coding

Two researchers performed the literature screening and coding task, with a third researcher to reconcile disagreements. Literature screening involves removing irrelevant or duplicated papers. To be more specific, if a paper mentions "composite" in its abstract but the "composite" does not refer to a material, the paper is excluded. Literature coding has three steps. (1) Identify the major topic of each paper from its title and abstract. (2) Combine similar topics to reduce the number of topics. (3) Categorise topics according to their closeness of discipline.

3 LITERATURE STATISTICS

3.1. Basic statistics

A total of 274 papers were retrieved from CNKI, while 148 were retrieved from Web of Science. After screening, irrelevant papers were excluded, leaving 222 and 86 papers, respectively, covering the years 1996 to 2017.

3.2. Research topics

The major topic of each paper was first identified, then combined, and finally categorised according to their closeness in discipline. For MD simulation papers, 9 topics were summarised and classified into 3 groups. Group 1 is physical property, including elasticity and plasticity, interfacial strength, viscoelasticity, and glass transition. Group 2 is physical process, covering molecular transfer and heat transfer. Group 3 is conformation, involving dispersion and assembly, defect and dislocation, and phase transfer and crystallisation.

Figure 1 reports the distribution of each MD simulation topic. Elasticity and plasticity, interfacial strength, molecular transfer, and dispersion and assembly are the 4 most studied topics. These are all typical and important

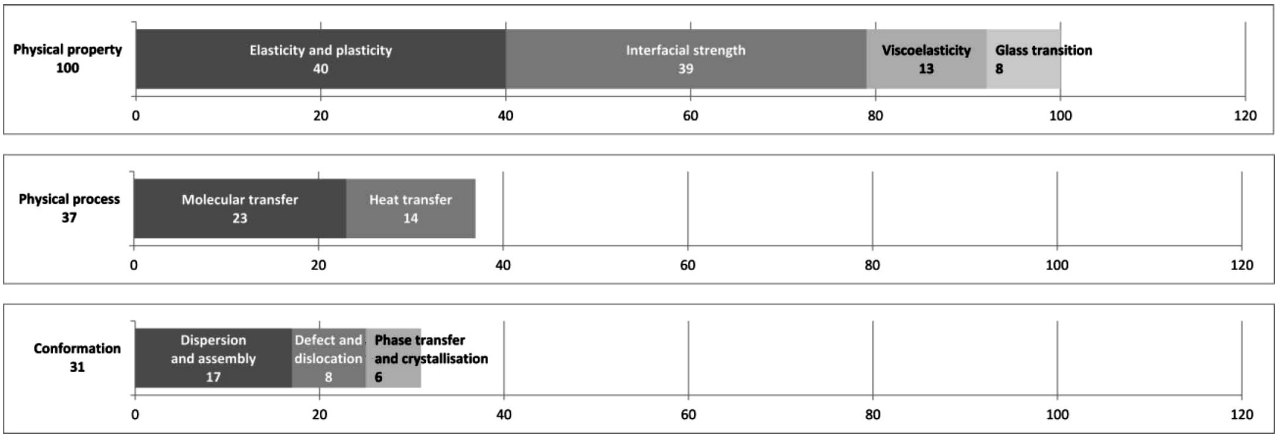

Figure 1: Topic distribution of MD simulation papers

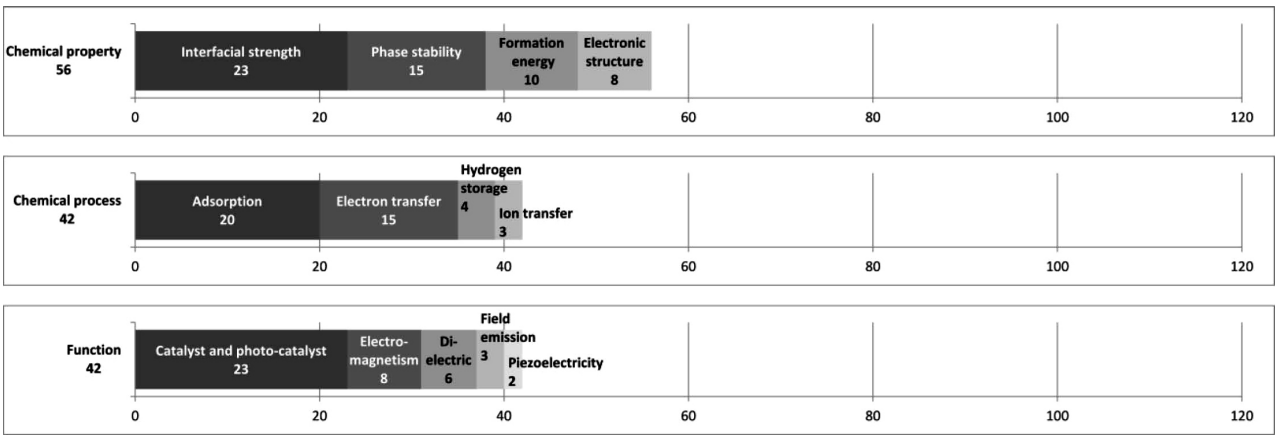

Figure 2: Topic distribution of ab-initio calculation papers

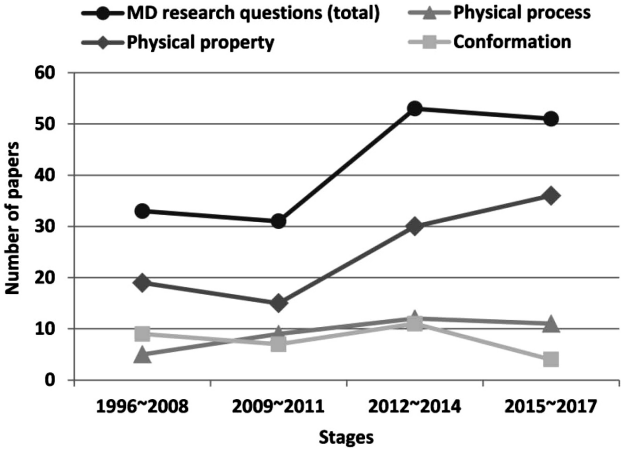

Figure 3: Topic trend of molecular dynamics simulation papers

molecular level problems that are relatively easy to model and straightforward to demonstrate.

Similarly, 13 ab-initio calculation topics and their numbers are displayed in **Figure 2**. Group 1 is chemical property, incorporating interfacial strength, phase stability, formation energy, and electronic structure. Group 2 is chemical process, including adsorption, electron transfer, hydrogen storage, and ion transfer. Group 3 is function, covering catalyst and photo-catalyst, electromagnetism, dielectric, field emission, and piezo electricity. Among them, interfacial strength, adsorption, and catalyst and photo-catalyst are the most popular.

3.3. Research trends

Besides the distribution of topic over disciplines, the coding process also reveals the evolution of topics over time. For each topic group, the number of papers therein was summed according to their year of publication. The years were divided into 4 stages, namely 1996–2008, 2009–2011, 2012–2014, 2015–2017. **Figure 3** shows the topic trend of MD simulation papers. The increment of the number of MD simulation studies stopped growing during 2015–2017. More specifically, whereas there is still a growing increment of physical property studies, new papers discussing physical process and conformation are reducing, indicating the maturity of MD simulation in solving these two problems, which results in fewer reports.

The topic trend of ab-initio calculation papers is plotted in **Figure 4**. Despite the decrease of new papers focusing on chemical process, the popularity of chemical property characterisation, functional application, as well as ab-initio calculation as a whole, is constantly growing. Therefore, future composite studies are expected to rely more on ab-initio calculations than molecular dynamics simulations.

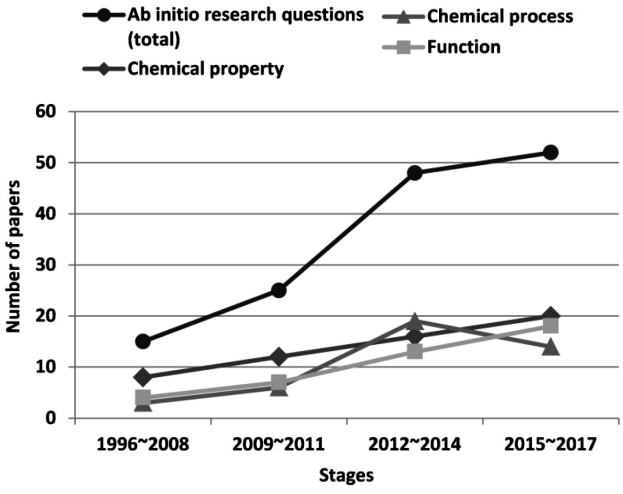

Figure 4: Topic trend of ab-initio calculation papers

4 MD SIMULATION HIGHLIGHT

In this section, a selection of the MD simulation studies is highlighted, which covers the aforementioned 9 topics.

4.1. Elasticity and plasticity

Elasticity is the ability of a material to resist geometric deformation, whereas plasticity describes the state of the mechanically loaded material that undergoes unrecoverable deformation. These are the fundamental properties of composite materials. The MD simulation starts with preparing a piece of material to be loaded, which normally contains several hundred atoms, followed by deforming the material in a tensile, shear, or compressive manner,[7–9] and ends with recording the resultant stress. Typical elastic and plastic properties and behaviours include Young's modulus, bulk modulus, shear modulus, Poisson's ratio, yield stress, yield strain, compressive strength, softening and hardening, and fracture strain.[10–15] Buckling and negative stiffness are also studied.[16,17]

4.2. Interfacial strength

The interface is ubiquitous in a composite material. Interfacial strength is the maximum load-carrying capability of the boundary of two constituents against separation load. The separation load is either normal to the interfacial plane, or tangential, such as fibre pull-out.[18–20] The simulation first builds the atomistic model of the studied interface, then deforms it in a tensile or shearing form, and finally measures the load displacement response. In this way, the interfacial strength and energy are obtained. By shearing the interface, researchers have further studied its friction and abrasion properties.[21,22] There is yet a simpler approach to study the composite interface by means of calculating the difference of free energy.[23,24] However, only interfacial energy can be obtained in this way, with the strength information missing.

4.3. Molecular transfer

Molecular transfer investigates the diffusion of gas or liquid molecules into, within, and out of a medium, which can be a membrane, a nano-tube, or a bulk.[25–27] Accurately predicting the molecular-transfer properties helps researchers design and optimise gas and liquid separation materials.[28–30] The diffusion simulation can be either free due to Brownian motion or compelled driven by pressure difference. Either way, the simulation first establishes the molecular framework of the diffusion media, then places a number of gas or liquid molecules into the framework, and finally observes the trajectory of these molecules under controlled temperature and pressure. The most widely used index to characterise diffusion is the mean square displacement,[31] which measures the distance over which a molecule travels within the simulation time window.

4.4. Dispersion and assembly

Composite synthesis always involves the compatibility,[32,33] dispersion,[34,35] aggregation,[36,37] and assembly[38,39] of materials. These conformational processes are critical in achieving ideal performance for the ultimate mixture. The corresponding MD simulation begins with situating the constituents in their initial position and orientation, followed by relaxing the system to reach minimum energy, and ends with quantifying the conformation using statistical tools. Usually, a subsequent simulation is performed to validate whether the optimised conformation indeed contributes to improved thermal or mechanical properties.

4.5. Other minor topics

4.5.1. Viscoelasticity

Viscoelasticity describes the nonsynchronous variation of stress and strain, resulting in relaxation, creep, or damping properties of viscoelastic materials. Industry has been keen on applying damping composites to absorb excessive vibration energy. Meanwhile, preventing composite structural failure from relaxation or creep is also of great importance. All these viscoelastic behaviours can be simulated using MD by controlling the profile of the stress and measuring the change of strain, or vice versa.[40–44]

4.5.2. Glass transition

Glass transition is the change of a material from a glassy state to a rubbery one when the temperature increases from below to above a certain temperate (range), or glass transition temperature. In the glassy state, the material is more rigid, whereas in the rubbery state, the material is more easy to deform. Glass transition is common for polymer and polymer-based composites. The MD characterisation of a material's glass transition is realised by capturing the sudden change of the volumetric- or diffusion-related property over a temperature sweep.[45–46]

4.5.3. Heat transfer

Heat transfer is a common phenomenon in composite applications,[47,48] whether to improve the heat exchange to reduce the energy loss,[49] or to arrest heat to concentrate energy.[50] In both situations, the simulation is performed by first preparing the material or interface to be studied, then configuring the temperature inside the material and on the boundary, and finally examining the evolution of the temperature field.

4.5.4. Defect and dislocation

A defect is one kind of imperfection in a crystalline composite that can lead to degraded mechanical performance. A dislocation is another kind of crystal imperfection that forms when mechanically loaded. Both defect and dislocation, after inclusion or initiation, can grow, displace, aggregate, or heal upon further loading.[51–54] Therefore, in order to maintain a material's strength and toughness, it is very necessary to study the behaviour, mechanism, and consequence of defect and dislocation.[55–57] To this end, in MD simulation, the crystal structure of the studied material is established, with a defect inserted if this applies. Afterwards, the material is mechanically deformed, and the crack is expected to initiate around the defect or the dislocation. By observing the failure mode, and subsequently introducing defect-eliminating or crack-stopping mechanisms, the material can reach optimal performance.

4.5.5. Phase transfer and crystallisation

Phase transfer, especially crystallisation, happens in composites usually when the temperature changes over a pivotal value.[58,59] In such a process, a relatively large amount of heat is absorbed or released, which is useful in heat- and temperature-management applications.[60,61] A MD simulation for phase transfer starts from building the crystal structure of the material(s), goes on with adjusting the temperature, and finishes by observing the appearance, disappearance, separation, or coalescence of the phases.

5 AB-INITIO CALCULATION HIGHLIGHT

This section highlights the selection of the ab-initio studies, covering the aforementioned 13 topics.

5.1. Interfacial strength

Interfacial strength is the most frequently studied topic for ab-initio composite studies. Unlike a MD simulation (see Section 4.2), an ab-initio calculation, albeit less computationally efficient, explores not only the separation energy of the interface, which is realised by calculating free energy,[62,63] but also the intrinsic mechanism of interfacial bonding by means of electron

level analysis, incorporating chemical bond population, atomic relaxation, and charge distribution.[64–68]

5.2. Adsorption

Adsorption is the accumulation of gases, liquids, or solutes on the surface of a solid or liquid. Adsorption is usually the first step of a chemical reaction that happens on a composite surface. The adsorbent can be a proton, an atom, a radical, a gas molecule, or a liquid molecule.[69–74] Moreover, an ab-initio calculation can also deal with interface or hydrophilicity problems in a more meticulous way.[75,76] An ab-initio adsorption calculation is similar to an interfacial strength calculation, which mainly investigates the difference of the total free energy after adsorption.

5.3. Catalyst and photo-catalyst

A catalyst is a material that can reduce the energy barrier of a chemical reaction and thereby accelerate the reaction. To produce the catalysing effect, the material needs to have an elaborate electron structure such that the reactant can adsorb easily; the intermediate product can move freely, and the resultant can leave without lingering.[77–81] A composite allows customising of the electron structure by carefully combining the constituents. A photo-catalyst is a special kind of catalyst that has a finely tuned band gap, sometimes called a heterojunction, such that the electron-cavity configuration can produce photoabsorption or photoresponse.[82–86]

5.4. Other minor topics

5.4.1. Phase stability

Metal composites have new phases formed during alloying, doping or oxidation.[87–91] An accurate estimation of the stability of these phases will benefit the design and synthesis of metal composites. An ab-initio calculation is able to compare the free energy of all possible interphases, eliminate the less probable ones, and recommend the most likely compositions.

5.4.2. Formation energy

Formation energy is the energy required to form a new composite material from its previous state by sintering, oxidation, in-situ reaction, precipitation, or other synthesising methods.[92–98] A lower formation energy indicates easier formation. An ab-initio formation-energy calculation is also viable by computing the difference in the free energy before and after formation.

5.4.3. Electronic structure

The electronic structure can provide the fundamental explanation to most chemical processes. Therefore, a calculation of the conduction band, valence band, band gap, density of state, and certain spectrums has been a basic and important practice in ab-initio studies.[99–102]

5.4.4. Electron transfer

The electron transfer process in a composite determines the thermal and electrical conductivity of the material.[103–105] Election transfer can happen in a crystal composite, on the surface of a composite, or across the interface between constituents.[106–108] By investigating the electronic structure of the different transfer passages using an ab-initio calculation, the conductivity of the materials is compared.

5.4.5. Hydrogen storage

Efficient hydrogen storage is crucial for the mass utilization of hydrogen energy, which features reproducibility and zero pollution. A hydrogen-storage solution other than a high-pressure vessel is via material-based mechanism involving metal atom-doped nano tube, nano plate, or covalent organic framework.[109–111] Material-based hydrogen storage is basically an adsorption problem.[112] Consequently, by calculating the decrease in the total free energy after hydrogen adsorption, the ability of the adsorbate is quantified.

5.4.6. Ion transfer

Ion transfer in composites is found in a composite-based lithium ion battery, where the lithium ion is inserted or extracted from the anode, cathode, or electrolyte materials made of composites.[113–115] An ab-initio calculation facilitates the characterisation of the lithium ion migration channel, such that the material can be optimised to guarantee the least ion transfer resistance.

5.4.7. Electro-magnetism

Composite electro-magnetism is useful in data storage and many other applications.[116] Electro-magnetism manifests as diamagnetism, ferromagnetism, multiferroics, ferroelectricity, and electronic controlled magnetism.[117–119] Electro-magnetism results from unpaired electrons or from local defects.[120,121] By inspecting the density of state and electron spinning using an ab-initio calculation, the electro-magnetism of composite materials can be characterised.

5.4.8. Dielectric

Composites with excellent dielectric properties are potential candidates for insulators.[122,123] The dielectric properties of a material mainly refer to the intensity of polarisation and the breakdown strength when subjected to an electric field.[124,125] An ab-initio calculation is able to examine the change of the electronic orbit or the covalent bond distribution of a material in an electric field,[126] and thereby obtain the dielectric properties.

5.4.9. Field emission

Field emission is the emission of electrons from a cathode composite material when subjected to a strong electric field. It is evaluated by the number of electrons per unit time, and can be characterised by the binding

energy, ionization energy, and work function, which are computable using an ab-initio calculation.[127–129]

5.4.10. Piezoelectricity

Piezoelectricity refers to the generation of electricity or of electric polarity in dielectric crystalline composites subjected to mechanical stress, or the generation of stress in such crystals subjected to an applied voltage.[130] Hardness and piezoelectric constant are the two most important properties of a piezoelectric material.[131] An ab-initio calculation can perform elastic constant and energy band simulation, which enables the prediction of the hardness and the piezoelectric constant.

6 CONCLUSIONS

Quantifying the phenomenon and probing the mechanism of composites by means of a MD simulation and/or an ab-initio calculation are promising in terms of feasibility and efficiency. This paper analyses relevant papers using literature coding and summarises the distribution and evolution of segmented research topics. The findings suggests that:

(1) For a MD simulation, elasticity and plasticity, interfacial strength, molecular transfer, and dispersion and assembly are the 4 most studied topics.

(2) For an ab-initio calculation, interfacial strength, adsorption, and catalyst and photo-catalyst are the most popular topics.

(3) Future composite studies will focus more on the ab-initio method, especially chemical property prediction and functional applications.

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