

A Framework for Visualizing the Dynamic Events of Carbon Nanocomposites using Virtual and Augmented Reality Tools

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Abstract: Atomic interactions pertaining to carbon-nanocomposites can be elusive and hard to comprehend, and as such great benefit can be gained through a visualization of these interactions within a virtual or augmented reality setting. In this paper, we present a framework that can be used for Material Science research and education incorporating topics related to the dynamics in nanomaterials. We developed the proof of concept implementation of this framework for Virtual Reality (VR) and Augmented Reality (AR) settings using the Unity game engine. Throughout this paper, we discuss our framework as well as the related user experiences and performance measurements we gathered when using our framework with the Google Daydream, HTC Vive, and Microsoft HoloLens in introducing scientists to the use of AR and VR as a tool for nanocomposite and molecular dynamics research.

1 INTRODUCTION

Carbon-nanocomposites have garnered more attention over the years due to their special properties like low density, high specific surface area, and thermal and mechanical stability (Krolow, 2013). They are used in various areas including batteries, biomedical technology, and structural components (Baughman, 2002). Carbon-nanocomposites have gathered interest due to a variety of reasons, including having a high elastic modulus and tensile strength being just two among many others (Arash, 2013). With this sudden popularity, comes the need for proper Molecular Dynamics (MD) simulation tools to aid in the research of these nanocomposite materials. These tools are important, as carbon nanotubes and nanocomposites in general are extremely difficult to study due to their size and their atomic nature. MD simulation tools help researchers to better understand the properties of carbon nanotubes (CNT) as well as how they will react under certain circumstances. One such circumstance that is of great interest to many researchers, is how CNT react under various conditions when subjected to the process of oxidation. Oxidation poses a challenge towards the use of CNT because oxygen molecules will bind to carbon molecules located within imperfections in the carbon nanotube structure and cause the nanotube to slowly decay through a process

of fraying and decomposition (Zhang, 2003). These imperfections can be difficult to detect and are typically common at the edges of a carbon nanotube. In order to bring greater flexibility to the study of these CNT in virtual and augmented reality, we developed a framework to better understand how carbon-nanocomposites react to oxidation. Researchers may upload data related to reactions they may be currently researching, and view them within virtual or augmented reality settings on a variety of different devices, e.g. Google Daydream, Microsoft HoloLens, as well as view them concurrently with multiple other researchers. This paper aims to present our generic framework for implementing this system of nanocomposites visualization and to increase the flexibility of the evaluation of nanocomposites.

The rest of the article is organized as follows: Previous initiatives and tools to visualize Molecular Dynamics simulation in VR/AR environments is highlighted in Section-2. Our proposed framework and relevant implementation details are provided in Section-3. Sections 4 and 5 contain the device-specific performance of our proof-of-concept framework implementation and end user survey results. Finally, we highlight our observations based on data collected from performance and survey results and the future direction of our ongoing work in Section-6.

2 RELATED WORKS

Research into applications of VR in relation to MD simulation has been undertaken in the past. In 1998 (Ali, 1998), researchers created their own set of VR hardware, labelled as the Cave Automatic Virtual Environments (CAVE), as no set of VR tools existed at the time that were commercially available and allowed for an easy development process. They then proceeded to create a software application which served as the MD simulation framework which was only compatible with the CAVE system.

More current research has also been undertaken in an attempt to realize a VR software framework for MD simulation which is compatible with modern, more commercially available VR tools and hardware systems. In one such study published in 2018 (O'Connor, 2018), researchers created a MD simulation framework for use with the HTC Vive which allowed for the real time simulation of atomic structures undergoing MD. This research, while limited to only one set of VR tools (the HTC Vive), demonstrates the incredible potential of MD simulations within a VR Environment when paired with powerful computational assets made available through modern technologies, like cloud computing.

Along with research studies regarding MD simulations, commercial applications also exist with the aim of providing an educational framework for the study of atomic molecules as well as to improve research capabilities.

MEL Science (melscience.com) is a company that specializes in educating children on the topic of chemistry. The company has created a VR application called the MEL Chemistry app which allows users to view chemical models. Although the application presents atomic structures to the user, these structures are static and do not move. The application is heavily catered towards students at the primary education grade level and does not contain robust tools for the study of more detailed chemical models for researchers.

EduChemVR is a start-up company based out of Sweden that also specializes in molecular and atomic education. The company has recently embarked on an endeavour to create applications to educate children on these topics and has, as such, created a VR application for students called Learning Carbons VR. This application presents users with static models of various carbon-based atomic structures. The application was developed using the Unity Game Engine and utilizes a Bluetooth gamepad controller for movement and Google Cardboard for displaying the atomic structures. Like MEL Chemistry, Learning Carbons VR is also

focused towards primary education grade level students and does not contain robust tools for the study of more detailed molecular models (educhem-vr.com).

LAMMPS is a fully realized MD simulation engine package created by Sandia National Laboratories (Plimpton, 1995). The program will produce atomic trajectory information documenting the movement of the individual atoms within the simulation box. Each trajectory records the movements for every 2 femto-seconds. The format of the LAMMPS results however is typically not compatible with VR devices, even though it does possess the ability to simulate complex, large scale chemical reactions involving thousands of individual atoms. We utilize LAMMPS to generate the data necessary for the visualization of atoms and molecular structures within our framework.

While the use of VR tools to simulate MD has maintained high levels of interest throughout the years, it is still very much a burgeoning field, especially when dynamic processes are of interest. As a side effect, access to frameworks for viewing MD simulations within VR has remained somewhat stagnant and researchers are often limited to a narrow scope of hardware from which to choose from. Taking notice of this issue, our framework aims to expand the range of VR tools available to researchers hoping to utilize said tools for MD simulations. Compared to the existing works cited in the literature, our framework has also expanded MD simulations to the realm of AR with the same initiative to enable a broad set of tools and hardware sets for researchers.

3 PROPOSED FRAMEWORK AND IMPLEMENTATION

In Figure-1, we present our proposed framework for a streamlined system to study MD simulations. The framework's ease of use and ability to be easily integrated into a research pipeline is enhanced by the fact that the application is compatible with a wide range of different VR and AR platforms. This enables researchers to be able to view a simulation in a variety of different VR or AR settings and does not restrain the researcher to a single device in which they must view their simulations. On top of this, the framework enables researchers to view any simulation concurrently with other researchers and makes this experience available across platforms. Therefore, researchers are less limited by the devices they have available and are able to take a more team centred approach towards their research if they so desire.

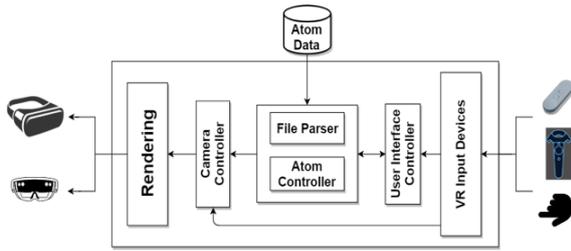


Figure 1: Our framework for CNT VR/AR simulation.

The proposed framework takes two inputs - simulation data created using LAMMPS and user interaction input collected via input devices associated with the various VR and AR hardware. The user input information fed into the system is used to allow a user to interact with any given User Interface (UI) and to allow for a user to control the camera when viewing a simulation.

The framework accepts simulation data from both cloud hosted databases and local file systems. In a single user setting, a user may upload their simulation data to a repository and then select the simulation from the list of available data. In a multi-user setting, users need the host-server (a user hosting the simulation) to select and run the simulation they would like to view and then other participants can join the same simulation remotely.

The simulation data is fed into a file parser which interprets the data for the given simulation and generates atoms based on this data, allocating the information gathered from the data to each atom's control script which then dictates the behaviour of the atom throughout the simulation.

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c  o
  1.000000000000
24.595100402832    0.000000000000    0.000000000000
0.000000000000    21.299999237061    0.000000000000
0.000000000000    0.000000000000    20.000000000000
190 8
Direct
0.024899675093    0.922650294153    0.151026499271
0.024896015705    0.989335234354    0.150835001469
0.074908417395    0.022680283125    0.150651502609
0.074906381709    0.089364323660    0.150402998924
0.124924068912    0.989340428074    0.150704002380
0.174934020509    0.022686386305    0.150560998917
0.174931597073    0.089370424042    0.150359499454
0.224951310268    0.922661039779    0.150792002678
0.224948460308    0.989346069527    0.150634002686
    
```

Figure 2: Molecular simulation data format.

In Figure-2, we show a snippet of one of our sample data sets of a molecular simulation generated by LAMMPS. The data set indicates the type of atoms present within the simulation as letters located at the top of the simulation file. C and O are present within this simulation standing for Carbon and Oxygen. The data set also shows the simulation matrix specifications

located just below the atom types present in the simulation and indicates below the matrix, the number of atoms of each type that are in the simulation. The number of atoms present, in this case 190 and 8, are written in the same order as the letter types at the top of the simulation file. In other words, 190 carbon atoms will be generated within the simulation along with 8 oxygen atoms. After this information is displayed in the data set, the word “Direct” is used to indicate the positional data of each atom present within the scene for a single frame. The atom data is always listed in the same order and is mapped to the atoms as they are listed in the atom types and numbers section of the data set. For example, in this data the first 190 sets of positional data correspond to carbon atoms whereas the last 8 correspond to oxygen atoms, following the ordering of the listed atom types. Lastly, the data set repeats this format for every frame that was simulated within LAMMPS, only changing the positional data within the “Direct” section of the data for each frame.

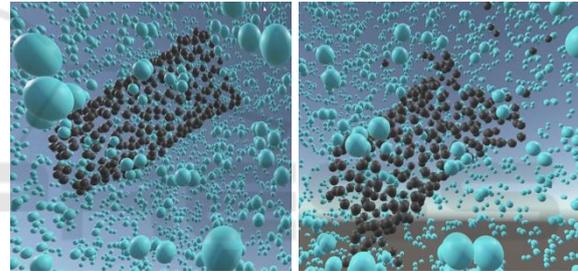


Figure 3: Simulation of carbon nanotube undergoing oxidation. Left: Initial stage, Right: Structural fraying.

Once the data is processed, the user is then able to control all aspects of a simulation through the UI and to control the camera positioning through the camera controller. After the initial set up, the camera data will be used to render the simulation, atoms, and UI. The proof-of-concept implementation of our proposed framework in Unity (unity3d.com) goes as follows:

1. Upon entering the application, the user will be presented with a menu and will utilize the various input devices associated with each of the Virtual or AR tool sets they are using to send data regarding their input to the system.
2. Input data sent into to the system will then be interpreted to allow for the user to interact with the given User Interface (UI) as well as to control the camera within the application once the simulation starts.
3. The user will then be able to interact with the UI to select whether or not they would like to view a simulation by themselves or with other users.

4. After making this selection, if the user chooses to view a simulation by himself then the user will be presented with a list of the available simulation data sets from which to choose from. If the user chooses to view a simulation with other users then they will be connected to a dedicated server and be able to view whichever simulation is currently running on this server.
5. Users also have the ability to upload a simulation data set generated by LAMMPS to a public website repository so that the simulation will be made available to be viewed within the application or to request that the dedicated server begin running a specific simulation dataset that the user would like to view with other users.
6. Once a simulation is selected to be viewed, the simulation data will be retrieved from the website repository and subsequently parsed and interpreted by the application. This process takes place on the user's system only in the case of a single user simulation due to the fact that the initial processing for a multi-user simulation is handled by the host-server.
7. Once a simulation dataset has been parsed and interpreted, data pertaining to atom behaviour is allocated to each individual atom object and the simulation begins running. If a user has joined a multi-user session, the server simply sends this atom behaviour to the client session of the user.
8. During the simulation, the user's camera renders the simulation (see Figure 3) and the user is given control of the camera to enable them to move around the simulation. In a multi-user setting, the only user allowed to manipulate the playback of the simulation is the user who has been assigned the role of "Lead" upon connecting to the server.
9. When a user is finished viewing a simulation, they can utilize the UI to exit the simulation they are currently viewing and will be returned to the start menu wherein the process will proceed from step 1.

4 SYSTEM PERFORMANCE

Device performance when using our framework was gathered via the frame rates measured while each device simulated different molecular processes containing different numbers of atoms (see Figure-4). Due to the Google Daydream's utilization of mobile devices and smartphones, it is limited in the amount of processing power as it has to perform calculations on large amounts of data. This was also an issue present within the Microsoft HoloLens as its onboard

processor is not powerful enough to render large data sets when not tethered to a computer. Because of this, for datasets with a number of atoms larger than 260, the Google Daydream and Microsoft HoloLens were unable to be utilized. For these larger datasets the HTC Vive was utilized which must remain tethered to a computer for processing. This allowed for the simulation of much larger data sets. The range of data sets that were tested for the various devices ranged from 198 atoms to 10,000 atoms.

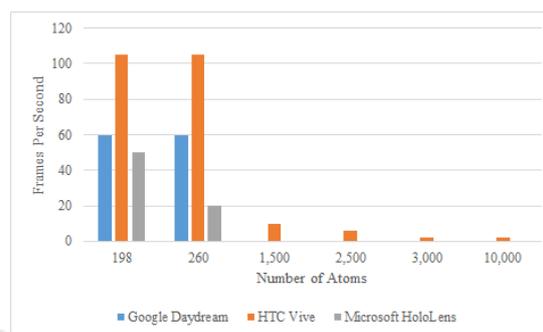


Figure 4: Framerate performance by number of atoms.

4.1 Google Daydream

The testing and development phases for the mobile and smartphone version of our application were performed on the Google Pixel 2. The Google Pixel 2 performed best when the data set contained trajectory data for 300 atoms or less. For data sets that contain more than 300 atoms, the Google Pixel 2 could take up to a minute or longer to transition into the scene containing the simulation. At 1000 atoms or more, the Google Pixel 2 consistently crashed and would not enter the simulation. This may be due to a failsafe mechanism on the phone that will not allow a program to lock up for more than a handful of minutes. It is also worth noting that even if the Google Pixel 2 could have rendered the simulation scene, it may not have been able to simulate it in real time without freezing or having a very low frame rate. Despite these limitations, the Google Daydream implementation has the unique advantage of making the program portable and any user should be able to use the application provided they have the hardware.

4.2 HTC Vive

For the HTC Vive to run the data sets, a GPU that is as powerful or better than the Nvidia GTX 1060 and have an Intel i5-4590 CPU or better is needed. All of our available datasets were able to run on the HTC Vive. We were unable to find an absolute cap wherein the

HTC Vive simply could not handle the number of atoms present within the simulation, however framerate would continue to decline as the number of atoms grew as can be seen in Figure-4.

4.3 Microsoft HoloLens

The Microsoft HoloLens makes use of a custom-built onboard processor and GPU in order to project 3D models into an AR environment. While the processor and GPU contained within the HoloLens are fairly powerful for a portable device of its kind, most of their processing power is spent computing various calculations to render and display 3D models within the environment as well as keep track of their position in world space. Therefore, the amount of processing power made available to the HoloLens for other tasks such as the calculations needed for our simulation was limited and performance issues began appearing in simulations with a number of atoms ranging as little as 260. It would appear that in this regard, the Microsoft HoloLens performed less optimally than the Google Daydream utilizing the Google Pixel 2. However, the Microsoft HoloLens provides the same advantages as the Google Daydream in that it is portable and able to be used from any location as long as an internet connection is established, as well as providing the unique added ability to project a simulation into the real world to be viewed in an AR setting.

5 SURVEY

A survey was composed to gain feedback on the effectiveness of the framework to be used in the development of VR and AR applications for MD simulation. The survey also provided us with information to better understand which device users found more user friendly and which device enabled them to better understand the interactions within the MD simulations. A total of 18 adult participants (not including the authors) were asked to participate in the survey. Any learning or fatigue effect was mitigated by randomizing which device users started with. There were no strenuous tasks for the participants to perform, except to interact with the user interface and move around their respective simulation.

5.1 Survey Questions

Questions used for the survey are as follows: Participants were given dichotomous, yes or no questions asking if they enjoyed their experience and if they have ever used a VR or AR device before. A

multiple answer question was given to determine past user experience with any of the devices used in the study, where users could choose any or all of the devices they had used before, the choices were HTC Vive, Oculus Rift, Smartphone VR, Microsoft HoloLens, or other.

A multiple-choice question was used to determine which device users enjoyed more and they were asked to provide a short answer for their choice. Participants were given Likert scale questions to gauge their ability to quickly learn and utilize the controls for each of the devices, where 1 represents having difficulty understand the controls and 5 represents having no difficulty understanding the controls.

Another Likert question was used to determine if the experience improved participant understanding of carbon nanocomposites, where 1 represents they disagree that the experience improved their understanding and 5 represents they agree the experience improved their understanding. One more Likert question was used to determine if the participants found the experience to be educational at all, where 1 represents not education and 5 represents very educational.

Finally, participants were asked short answer questions for what they enjoyed most about the experience, what they disliked, and for any other feedback in regards to the application.

5.2 Survey Results

The majority of participants (12 out of 18) have had experience with VR or AR devices before. When asked which devices the participants had used before, 7 answered HTC Vive, 7 answered Microsoft HoloLens, 1 answered Google Daydream, and 8 answered other.

For the question covering which device users enjoyed the most, 10 (55.6%) of the participants answered HTC Vive while the Microsoft HoloLens received 5 (27.8%) votes. Users reported the HTC Vive as the "most responsive" and "more immersive" than the Daydream or HoloLens.

As for the questions pertaining to the controls and ease of use of the devices, the Vive and Daydream had similar responses where 10 (55.6%) of the participants strongly agreed that the controls were easy to understand. For the HoloLens, 6 (33.3%) strongly agreed the controls were easy to understand, 5 (27.8%) agreed, 6 (33.3%) were in the middle, and 1 (5.6%) disagreed that the controls were easy to understand. Next, participants were asked about whether or not the experience was educational and whether or not the experience improved their understanding of carbon nano-composites. Overall, most of the participants

found the experience to be educational and that it improved their understanding of the structure of carbon nanocomposites. Eight (44.4%) strongly agreed that the experience was educational and that it helped improve their understanding of carbon nanocomposites, 6 (33.3%) agreed that it improved their understanding of carbon nanocomposites, 7 (38.9%) agreed that the experience was educational, and no one answered disagree or strongly disagree on either question. Participants gave suggestions for longer simulations, labels for the atoms, and more information in the scenes for what is being viewed.

Lastly, participants were asked to give short answers in regards to what they enjoyed about the experience, what they disliked, and for other comments that may be helpful to the developers. All but 1 participant, who responded "N/A", answered that they mostly enjoyed using the different devices. One participant stated, "I enjoyed being able to observe a complex phenomenon in a way that made it simple to understand." In regards to what users disliked about the experience, 4 reported motion sickness with the Vive and 5 reported general usability issues with the HoloLens.

6 CONCLUSIONS

In this paper, a framework for researching molecular dynamic processes within virtual and augmented reality settings was presented. We demonstrated that our framework provides researchers an easily accessible and robust tool for visualizing the interactions within VR and/or AR settings. Based on the survey results, it is evident that the participants were able to make use of our application to enhance their understanding of the atomic interactions they were witnessing along with the structure of carbon nano-composites. It is worth noting that many of the criticisms the survey participants mentioned or the issues they were encountering were mostly due to the limitations of the device they were using as opposed to the framework we were showcasing to them. Despite these issues, the survey demonstrated that the framework we created is useable in all of the VR and AR settings we presented to the participants. Another significant finding of our survey was that many of the users stated that they found the VR and AR aspects of our framework when viewing the MD simulations served to enrich the viewing experience. Many participants mentioned that the ability to navigate a MD simulation in a fully immersive 3D setting helped them to better understand both the micro-level atomic reactions and the macro-level molecular dynamic

events themselves. This illustrates the potential benefits of our framework to enable researchers to gain a more 3D understanding of molecular dynamic events in AR/VR settings.

We aim to expand our current framework to allow for the real time simulation of molecular dynamics processes and are currently working on implementing a system in which users can interact with a given simulation even if all of the atomic events within the simulation are not being calculated in real time. We also plan on further developing the framework to allow for greater detail in regards to the atomic reactions taking place within any given simulation such as showing the bonding between atoms, temperature, atomic mass, and other relevant details of a CNT/MD simulation.

REFERENCES

- Krolow, M.Z., Hartwig, C.A., Link, G.C., Raubach, C.W., Pereira, J.S.F., Picoloto, R.S., Gonçalves, M.R.F., Carreño, N.L.V. and Mesko, M.F., 2013. Synthesis and characterisation of carbon nanocomposites. In *NanoCarbon 2011* (pp. 33-47). Springer, Berlin, Heidelberg.
- Baughman, R.H., Zakhidov, A.A. and De Heer, W.A., 2002. Carbon nanotubes--the route toward applications. *science*, 297(5582), pp.787-792.
- Arash, B., Wang, Q. and Varadan, V.K., 2014. Mechanical properties of carbon nanotube/polymer composites. *Scientific reports*, 4, p.6479.
- Zhang, J., Zou, H., Qing, Q., Yang, Y., Li, Q., Liu, Z., Guo, X. and Du, Z., 2003. Effect of chemical oxidation on the structure of single-walled carbon nanotubes. *The Journal of Physical Chemistry B*, 107(16), pp.3712-3718.
- Ai, Z. and Fröhlich, T., 1998, August. Molecular dynamics simulation in virtual environments. In *Computer Graphics Forum* (Vol. 17, No. 3, pp. 267-273). Oxford, UK and Boston, USA: Blackwell Publishers Ltd.
- O'Connor, M., Deeks, H.M., Dawn, E., Metatla, O., Roudaut, A., Sutton, M., Thomas, L.M., Glowacki, B.R., Sage, R., Tew, P. and Wonnacott, M., 2018. Sampling molecular conformations and dynamics in a multiuser virtual reality framework. *Science advances*, 4(6), p.eaat2731.
- Plimpton, S., 1995. Fast parallel algorithms for short-range molecular dynamics. *Journal of computational physics*, 117(1), pp.1-19.