# B. TECH. PROJECT REPORT

**On**

# UNDERSTANDING FAILURE OF CONCRETE STRUCTURES

**by**

**Namrata Singh**

**DISCIPLINE OF CIVIL ENGINEERING**

**INDIAN INSTITUTE OF TECHNOLOGY INDORE**

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# Understanding Failure of Concrete Structures

**A PROJECT REPORT**

***Submitted in partial fulfillment of the***
***requirements for the award of the degrees***
***of***
**BACHELOR OF TECHNOLOGY**
**in**
**CIVIL ENGINEERING**

***Submitted by:***
**Namrata Singh**

***Guided by:***
**Dr. Saikat Sarkar**
**Assistant Professor**
**Discipline of Civil Engineering**

# INDIAN INSTITUTE OF TECHNOLOGY INDORE

**Nov 2019**

# CANDIDATE’S DECLARATION

I hereby declare that the project entitled “**Understanding Failure of Concrete”** submitted in partial fulfillment for the award of the degree of Bachelor of Technology in ‘Civil Engineering’ completed under the supervision of **Dr. Saikat Sarkar, Assistant Professor, Discipline of Civil Engineering**, IIT Indore is an authentic work.

Further, I declare that I have not submitted this work for the award of any other degree elsewhere.

**Signature and name of the student(s) with date**

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# CERTIFICATE by BTP Guide(s)

**It is certified that the above statement made by the students is correct to the best of my/our knowledge.**

**Signature of BTP Guide(s) with dates and their designation**

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# Preface

This report on "**Understanding Failure of Concrete**" is prepared under the guidance of **Dr. Saikat Sarkar, Assistant Professor, Discipline of Civil Engineering, IIT Indore**.

In this BTP report I will describe my experiences during the 7th semester. The report contains an overview of the readings, simulations and findings during the semester. Writing this report, I also will describe and reflect my learning objects and personal goals that I had set. I have tried to discover the relationship between theoretical and practical type of knowledge and to bridge the gap between theoretical assumptions and practical necessities. With these objectives, I have made all possible efforts and the necessary investigations to submit this paper in an enlightened form in a very short time. I have tried my level best to eliminate errors from the paper. As I had to complete my internship within a short period of time so the study admits its limitations.

The report covers all the tasks completed keeping up with the minute details and their analysis. The simulation rendering images and analysis mechanical property graphs are attached step by step to give a better vision to the project. The report also elaborates on the future scope which can be pursued as an advancement of the current work. I have tried to the best of my ability and knowledge to explain the content in a lucid manner.

Under Dr. Saikat Sarkar's guidance, I am currently working on a manuscript of a paper titled " **Randomized Molecular Models of Cement and Concrete**" to be submitted in an International Journal.

# Acknowledgement

I would like to express my sincere gratitude to my BTP advisor and mentor, Dr. Saikat Sarkar who has given his valuable time and given me a chance to work on the interesting project. I would also like to thank him for supporting me during the completion and documentation of this BTP.

An eminent coder himself, he constantly encouraged me to face my fear of coding and his valuable experience and knowledge aided me in building my concepts and progress me in this project.

He has given me a vision to explore, learn, create and analyze new structures at the very basic levels which has helped me explore not only new opportunities but also my abilities. I am obliged that I was constantly encouraged and supported all the time during this project.

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# Abstract

Understanding and mitigating failure of structures has always been a major challenge for Civil Engineers. Given the complexity and arbitrary heterogeneity in Civil Engineering materials like concrete it is extremely difficult to get precise understanding about their behavior via brute force experiments. More over such experiments are costly. An alternative and probably preferred approach would be to perform molecular level computational studies on these materials. Concrete consists of C-S-H gel, aggregates and water in varied proportions. Even after efforts by many researchers, precise information about the molecular structure of concrete is still not quite known. As a part of this BTP project, I have proposed a randomized molecular model for the first time for concrete. The model accurately captures mechanical behavior of cement and concrete.

## List of Figures

# Chapter 1: INTRODUCTION

Structural failure is one of the most recurring and serious problems in Civil engineering worldwide which results in human, environmental and economic losses. Most of the studies specifically focus on prevention and prediction of structure failure by considering all possibilities in advance and using enhancements to prevent structure failure. Concrete is a composite material composed of fine and coarse aggregate bonded together with cement paste that hardens over time. It is an essential and primary constituent in most of the structures; hence, making concrete analysis an unavoidable step. As concrete is weaker in tension, it is observed that as concrete fails, the structure fails in tension.

Concrete Failure may occur due to various reasons: -

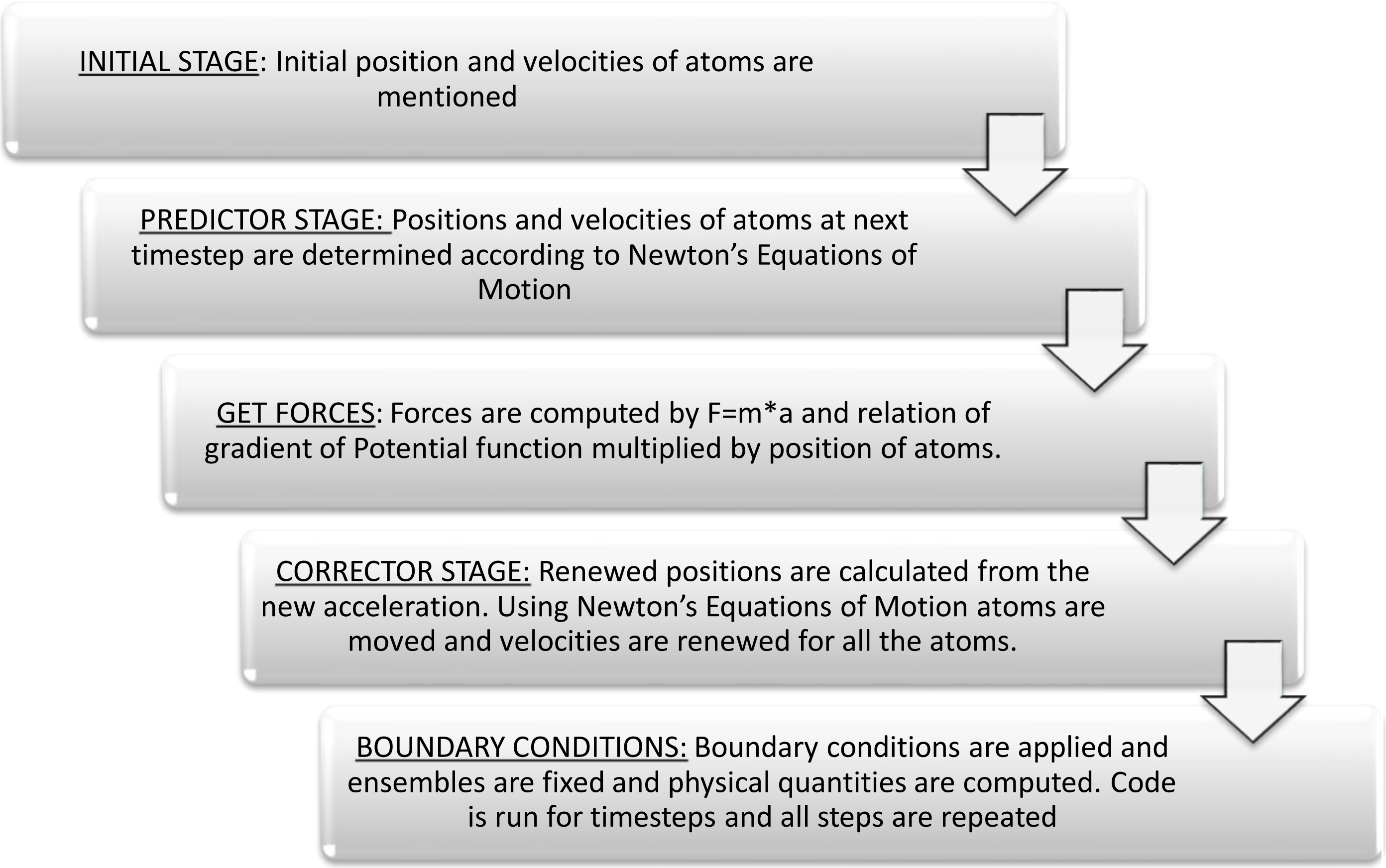
- Incorrect selection of materials
- Errors in design calculation and detailing
- Improper construction techniques and insufficient quality control and supervision
- Chemical attacks on concrete structures
- External mechanical factors

Most of these types of failures could be better understood if studied at atomistic or molecular level. Also, experimenting directly with any new material reinforcement could cost human expenses and resources while molecular view of new ideas could help one decide and predict the results in a very accurate manner of the new formed material.

Molecular dynamics (MD) is a simulation-based approach for analyzing the physical movements of atoms and molecules. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic "evolution" of the system. The trajectories of atoms and molecules are determined by numerically solving Newton's equations of motion for a system of interacting particles, where forces between the particles and their potential energies are often calculated using interatomic potentials or molecular mechanics force fields. The method is applied mostly in chemical physics, materials science, and the biophysics. Because molecular systems typically consist of a vast number of particles, it is impossible to determine the properties of such complex systems analytically; MD simulation circumvents this problem by using numerical methods. However, long MD simulations are mathematically ill-conditioned, generating cumulative errors in numerical integration that can be minimized with proper selection of algorithms and parameters, but not eliminated entirely.

For systems which obey the ergodic hypothesis, the evolution of one molecular dynamics simulation may be used to determine macroscopic thermodynamic properties of the system: the time averages of an ergodic system correspond to micro canonical ensemble averages. MD has also been termed "statistical mechanics by numbers" and "Laplace's vision of Newtonian mechanics" of predicting the future by animating nature's forces and allowing insight into molecular motion on an atomic scale.

## SIMPLIFIED SIMULATION ALGORITHM OF MOLECULAR DYNAMICS



INITIAL STAGE: Initial position and velocities of atoms are mentioned

PREDICTOR STAGE: Positions and velocities of atoms at next timestep are determined according to Newton’s Equations of Motion

GET FORCES: Forces are computed by F=m*a and relation of gradient of Potential function multiplied by position of atoms.

CORRECTOR STAGE: Renewed positions are calculated from the new acceleration. Using Newton’s Equations of Motion atoms are moved and velocities are renewed for all the atoms.

BOUNDARY CONDITIONS: Boundary conditions are applied and ensembles are fixed and physical quantities are computed. Code is run for timesteps and all steps are repeated

A simplified description of the standard molecular dynamics simulation algorithm, when a predictor-corrector-type integrator is used. The forces may come either from classical interatomic potentials(described mathematically as $F = -\nabla V(\hat{r})$) or quantum mechanical (described mathematically as $F=F(\psi(\hat{r}))$ methods. Large differences exist between different integrators; some do not have exactly the same highest-order terms as indicated in the flow chart, many also use higher-order time derivatives, and some use both the current and prior time step in variable-time step schemes.

Design of a molecular dynamics simulation should account for the available computational power. Simulation size (n = number of particles), time step, and total time duration must be selected so that the calculation can finish within a reasonable time period. However, the simulations should be long enough to be relevant to the time scales of the natural processes being studied. To make statistically valid conclusions from the simulations, the time span simulated should match the kinetics of the natural process. Otherwise, it is analogous to making conclusions about how a human walks when only looking at less than one footstep. Most scientific publications about the dynamics of proteins and DNA use data from simulations spanning nanoseconds ($10^{-9}$ s) to microseconds ($10^{-6}$ s). To obtain these simulations, several CPU-days to CPU-years are needed. Parallel algorithms allow the load to be distributed among CPUs.

In all kinds of molecular dynamics simulations, the simulation box size must be large enough to avoid boundary condition artifacts. Boundary conditions are often treated by choosing fixed values at the edges (which may cause artifacts), or by employing periodic boundary conditions in which one side of the simulation loops back to the opposite side, mimicking a bulk phase (which may cause artifacts too).

Microcanonical ensemble (NVE):

In the microcanonical ensemble [1], the system is isolated from changes in moles (N), volume (V), and energy (E). It corresponds to an adiabatic process with no heat exchange. A microcanonical molecular dynamics trajectory may be seen as an exchange of potential and kinetic energy, with total energy being conserved. For a system of N particles with coordinates X and velocities V, the following pair of first order differential equations may be written in Newton's notation as

$$F(X) = -\nabla U(X) = M\dot{V}(t)$$

$$\mathrm{V}(\mathrm{t}) = \dot{\mathrm{X}}(\mathrm{t})$$

The potential energy function U ( X ) of the system is a function of the particle coordinates X. It is referred to simply as the potential in physics, or the force field in chemistry. The first equation comes from Newton's laws of motion; the force F acting on each particle in the system can be calculated as the negative gradient of U ( X ). For every time step, each particle's position X and velocity V may be integrated with a simplistic integrator method such as Verlet integration. The time evolution of X and V is called a trajectory. Given the initial positions (e.g., from theoretical knowledge) and velocities (e.g., randomized Gaussian), we can calculate all future (or past) positions and velocities.

One frequent source of confusion is the meaning of temperature in MD. Commonly one has had experienced with macroscopic temperatures, which involve a huge number of particles. But temperature is a statistical quantity. If there is a large enough number of atoms, statistical temperature can be estimated from the instantaneous temperature, which is found by equating the kinetic energy of the system to $nk_BT/2$ where n is the number of degrees of freedom of the system and $k_B$ is the Boltzmann constant.

A temperature-related phenomenon arises due to the small number of atoms that are used in MD simulations. For example, consider simulating the growth of a copper film starting with a substrate containing 500 atoms and a deposition energy of 100 eV. In the real world, the 100 eV from the deposited atom would rapidly be transported through and shared among a large number of atoms ( $10^{10}$ ) with no big change in temperature. When there are only 500 atoms, however, the substrate is almost immediately vaporized by the deposition. Something similar happens in biophysical simulations. The temperature of the system in NVE is naturally raised when macromolecules such as proteins undergo exothermic conformational changes and binding.

### Canonical ensemble (NVT)

In the canonical ensemble, amount of substance (N), volume (V) and temperature (T) are conserved. It is also sometimes called constant temperature molecular dynamics (CTMD). In NVT, the energy of endothermic and exothermic processes is exchanged with a thermostat.

A variety of thermostat algorithms are available to add and remove energy from the boundaries of a MD simulation in a more or less realistic way, approximating the canonical ensemble. Popular methods to control temperature include velocity rescaling, the Nosé–Hoover thermostat, Nosé–Hoover chains, the Berendsen thermostat, the Andersen thermostat and Langevin dynamics. The Berendsen thermostat might introduce the flying ice cube effect, which leads to unphysical translations and rotations of the simulated system.

It is not trivial to obtain a canonical ensemble distribution of conformations and velocities using these algorithms. How this depends on system size, thermostat choice, thermostat parameters, time step and integrator is the subject of many articles in the field.

### Isothermal–isobaric (NPT) ensemble

In the isothermal–isobaric ensemble, amount of substance (N), pressure (P) and temperature (T) are conserved. In addition to a thermostat, a barostat is needed. It corresponds most closely to laboratory conditions with a flask open to ambient temperature and pressure.

### Generalized ensembles

The replica exchange method is a generalized ensemble. It was originally created to deal with the slow dynamics of disordered spin systems. It is also called parallel tempering. The replica exchange MD (REMD) formulation tries to overcome the multiple-minima problem by exchanging the temperature of non-interacting replicas of the system running at several temperatures.

## Potentials in MD simulations

A molecular dynamics simulation requires the definition of a potential function, or a description of the terms by which the particles in the simulation will interact. In chemistry and biology this is usually referred to as a force field and in materials physics as an interatomic potential. Potentials may be defined at many levels of physical accuracy; those most commonly used in chemistry are based on molecular mechanics and embody a classical mechanics treatment of particle-particle interactions that can reproduce structural and conformational changes but usually cannot reproduce chemical reactions.

The reduction from a fully quantum description to a classical potential entails two main approximations. The first one is the Born–Oppenheimer approximation, which states that the dynamics of electrons are so fast that they can be considered to react instantaneously to the motion of their nuclei. As a consequence, they may be treated separately. The second one treats the nuclei, which are much heavier than electrons, as point particles that follow classical Newtonian dynamics. In classical molecular dynamics, the effect of the electrons is approximated as one potential energy surface, usually representing the ground state.

When finer levels of detail are needed, potentials based on quantum mechanics are used; some methods attempt to create hybrid classical/quantum potentials where the bulk of the system is treated classically but a small region is treated as a quantum system, usually undergoing a chemical transformation.

## Empirical potentials

Empirical potentials used in chemistry are frequently called force fields, while those used in materials physics are called interatomic potentials.

Most force fields in chemistry are empirical and consist of a summation of bonded forces associated with chemical bonds, bond angles, and bond dihedrals, and non-bonded forces associated with van der Waals forces and electrostatic charge. Empirical potentials represent quantum-mechanical effects in a limited way through ad-hoc functional approximations. These potentials contain free parameters such as atomic charge, van der Waals parameters reflecting estimates of atomic radius, and equilibrium bond length, angle, and dihedral; these are obtained by fitting against detailed electronic calculations (quantum chemical simulations) or experimental physical properties such as elastic constants, lattice parameters and spectroscopic measurements.

Because of the non-local nature of non-bonded interactions, they involve at least weak interactions between all particles in the system. Its calculation is normally the bottleneck in the speed of MD simulations. To lower the computational cost, force fields employ numerical approximations. Chemistry force fields commonly employ preset bonding arrangements (an exception being ab initio dynamics), and thus are unable to model the process of chemical bond breaking and reactions explicitly. On the other hand, many of the potentials used in physics, such as those based on the bond order formalism can describe several different coordinations of a system and bond breaking.

## Pair potentials versus many-body potentials

The potential functions representing the non-bonded energy are formulated as a sum over interactions between the particles of the system. The simplest choice, employed in many popular force fields, is the "pair potential", in which the total potential energy can be calculated from the sum of energy contributions between pairs of atoms. Therefore, these force fields are also called "additive force fields". An example of such a pair potential is the non-bonded Lennard–Jones potential [3] (also termed the 6–12 potential), used for calculating van der Waals forces.

$$U(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^{6}]$$

where ε is the depth of the potential well, σ is the finite distance at which the inter-particle potential is zero, r is the distance between the particles, and $r_m$ is the distance at which the potential reaches its minimum. At $r_m$, the potential function has the value $-\varepsilon$. The distances are related as $r_m \approx 1.122\sigma$. These parameters can be fitted to reproduce experimental data or accurate quantum chemistry calculations. Due to its computational simplicity, the Lennard-Jones potential is used extensively in computer simulations even though more accurate potentials exist.

The $r^{-12}$ term, which is the repulsive term, describes Pauli repulsion at short ranges due to overlapping electron orbitals, and the $r^{-6}$ term, which is the attractive long-range term, describes attraction at long ranges (van der Waals force, or dispersion force).

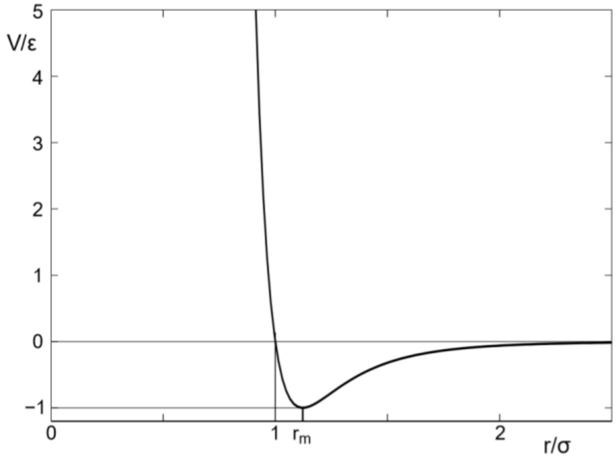


**Fig 1.1: A graph of strength versus distance for the 12-6 Lennard-Jones potential**

Differentiating the L-J potential with respect to r gives an expression for the net inter-molecular force between 2 molecules. This inter-molecular force may be attractive or repulsive, depending on the value of r. When r is very small, the molecules repel each other.

Whereas the functional form of the attractive term has a clear physical justification, the repulsive term has no theoretical justification. It is used because it approximates the Pauli repulsion well and is more convenient due to the relative computing efficiency of calculating $r^{12}$ as the square of $r^6$.

The L-J potential is a relatively good approximation. Due to its simplicity, it is often used to describe the properties of gases and to model dispersion and overlap interactions in molecular models. It is especially accurate for noble gas atoms and is a good approximation at long and short distances for neutral atoms and molecules.

The lowest-energy arrangement of an infinite number of atoms described by a Lennard-Jones potential is a hexagonal close-packing. On raising temperature, the lowest-free-energy arrangement becomes cubic close packing, and then liquid. Under pressure, the lowest-energy structure switches between cubic and hexagonal close packing. Real materials include body-centered cubic structures also.

The Lennard-Jones (12,6) potential was improved by the Buckingham potential (exp-6) later proposed by Richard Buckingham, incorporating an extra parameter and the repulsive part is replaced by an exponential function:

$$V_B = \gamma \, [\, e^{-(r / r1)} - (r_{0/} \, r)^6]$$

# Scripting Simulators and Softwares Used

1. LAMMPS
2. OVITO
3. Material Studio

LAMMPS: Molecular Dynamics simulation of nano-scale copper has been done using LAMMPS (*Large-scale Atomic/Molecular Massively Parallel Simulator*) [2]. It is a classical molecular dynamics simulation code designed to run efficiently on parallel computers which is an open-source code that models an ensemble of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, metallic, granular, and coarse-grained systems using a variety of force fields and boundary conditions. LAMMPS integrates Newton's equations of motion for collections of molecules, atoms, or macroscopic particles which interact by short- or long-range forces with a variety of initial and/or boundary conditions. For computational efficiency, LAMMPS uses neighbor lists (optimized for systems with particles that are repulsive at short distances, so that the local density of particles never becomes too large) to keep track of nearby particles. On parallel machines, to partition the simulation domain into small 3d sub-domains, it uses spatial decomposition techniques.

A LAMMPS input script has 4 parts: -

1. Initialization   2. Atom definition
3. Settings   4. Run a simulation

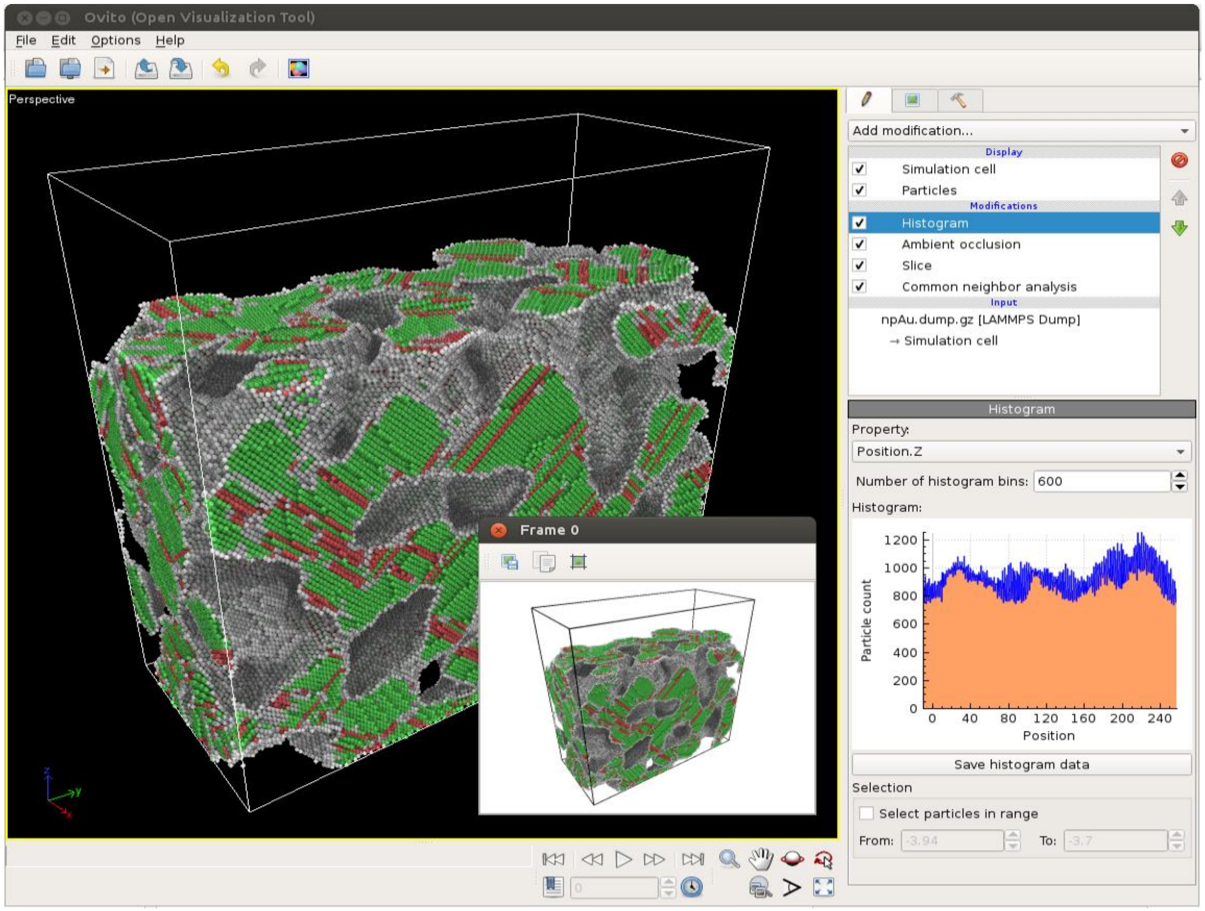
LAMMPS executes commands from an input script (text file), reading one line at a time. It exits when the input script ends. Every command causes LAMMPS to perform an action; it can read in a file, set an internal variable, or run a simulation. Generally, the ordering of commands in an input script is insignificant.

Precautions: -

1. LAMMPS reads the input script one line at a time and each command takes effect immediately when it is read, not after the complete text file is read.
2. A few commands are valid only when they follow other commands. A group command can only be used after the atoms are defined.
3. Sometimes a command X may use values set by command Y. This means command X must follow command Y in the input script if it is to have the required effect.

OVITO: OVITO makes molecular dynamics simulations visual. It is a visualization and analysis software for output data generated in molecular dynamics, atomistic Monte-Carlo and other particle-based simulations [4].

Data pipeline technology: OVITO as a data visualization and analysis solution provides a maximum of flexibility – and, at the same time, ease-of-use – to support one in extracting meaningful information from simulation outputs. To achieve this goal, it is based on a powerful data pipeline technology depicted below.



Property: Position.Z

Number of histogram bins: 600

☐ Select particles in range

From: -3.94 To: -3.7

Fig 1.2: (This figure is taken from OVITO website)

The software offers a wide range of basic visualization and analysis functions (building blocks), which one can assemble to a sequence of processing steps. These operations, which are all configurable, will then be applied to the simulation data in real-time by the software. The outcome of the data can be displayed on screen, may be rendered to an output image for publication, or exported to output data files.

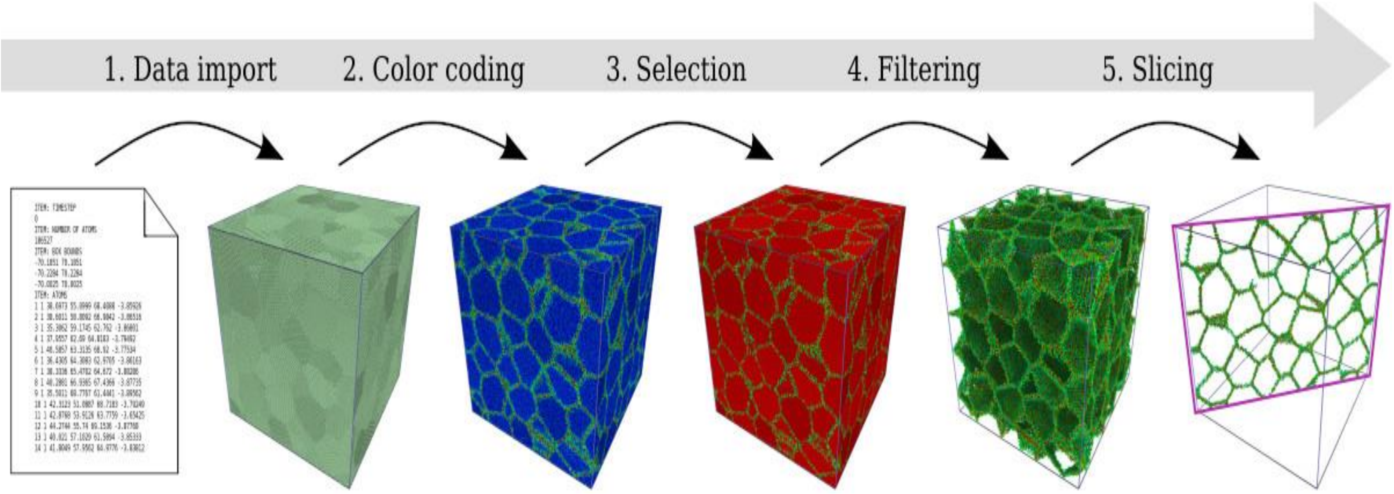


Fig 1.3 (This figure is taken from OVITO website)

The dynamic pipeline concept makes it possible to change and adjust the sequence of applied operations at any time. OVITO enables one to work in a non-destructive manner with a dataset as all manipulation steps can easily be revoked. One can adjust the order of filter and manipulation operations, their parameters, and also the input data itself –the program will re-evaluate the pipeline and update the display in real-time. The intelligent data caching and parallelization techniques implemented in OVITO works without interrupting the workflow.

MATERIAL STUDIO [5]: Materials Studio is a complete modeling and simulation environment designed to predict and understand the relationships of a material’s atomic and molecular structure with its properties and behavior. Using Materials Studio, researchers in many industries are engineering better performing materials of all types, including pharmaceuticals, catalysts, polymers and composites, metals and alloys, batteries and fuel cells, and more. Material Studio accelerates Innovation: Materials Studio enables materials scientists and research teams to develop new, better performing, and more cost effective materials faster and more efficiently than with test and experimentation alone. The software is very handy in creating molecular and atomic structures according to the user. Also, it corrects the structure with the help of smart inbuilt tools like *close contact, measure bonds, measure bond angles, check hybridization, etc.* Crystal Building and superstructures are just a click away which helps the users analyze the structure at a larger scale value. Many other properties like *layer* can be used to combine two structures of similar crystal type. Material Studio could be used as a visualization tool as well but mostly it helps convert atomic properties and positions to a data file.

NOTEPAD++: Notepad++ is a coding platform for different languages and LAMMPS coding is generally done by Notepad++. It is a light weighing software cum app that is user friendly and supports n number coding languages.

# CHAPTER 2: Contribution

## 2.1 PROJECT PROGRESS

- Shear Simulation of Nickel
- Tension Simulation of Copper upon application of Temperature Change
- Compression Simulation of Copper upon application of Temperature Change
- Compression simulation of Copper and Aluminum Alloy upon application of Temperature Change
- Unidirectional Failure of pure elemental Iron under Tension
- Study of Clinker Structures
- Study of CSH Gel
- Tension Simulation of CSH gel
- Analysis of CSH gel Mechanical Properties
- Study of Concrete
- Tension Simulation of Concrete Structure
- Compressive Simulation of Concrete Structure
- Analysis of Mechanical Properties of Concrete

# Chapter 3: Procedure, Observations and Results

## 1. ***Shear Analysis of Nickel: -***

I. LAMMPS input script

   a) Initialization: 3-D simulation block of 10*10*10 is defined with periodic boundaries.

   b) Atom Definition: FCC lattice is defined and the simulation box is divided into 3 parts- fixed, upper, mobile.

   c) Force Fields: Ni.meam potential file is called to define the atoms. meam potential is used to define Nickel atoms properties.

   d) Settings: Ensemble is fixed to nve, fixed region is set to force = 0.0 units in all three directions, upper region is set to unit velocity in x direction, mobile region is set to 300K and 10-unit velocity is set.

   e) Dump: The combined analysis is dumped in dump.shear at a time step of 100 and run for 3000 simulations.

II. The input script is run in command prompt in serial version which is side by side saved in a log.lammps file to be reviewed later

III. OVITO: The dump file is loaded in OVITO and the simulation is viewed with time.

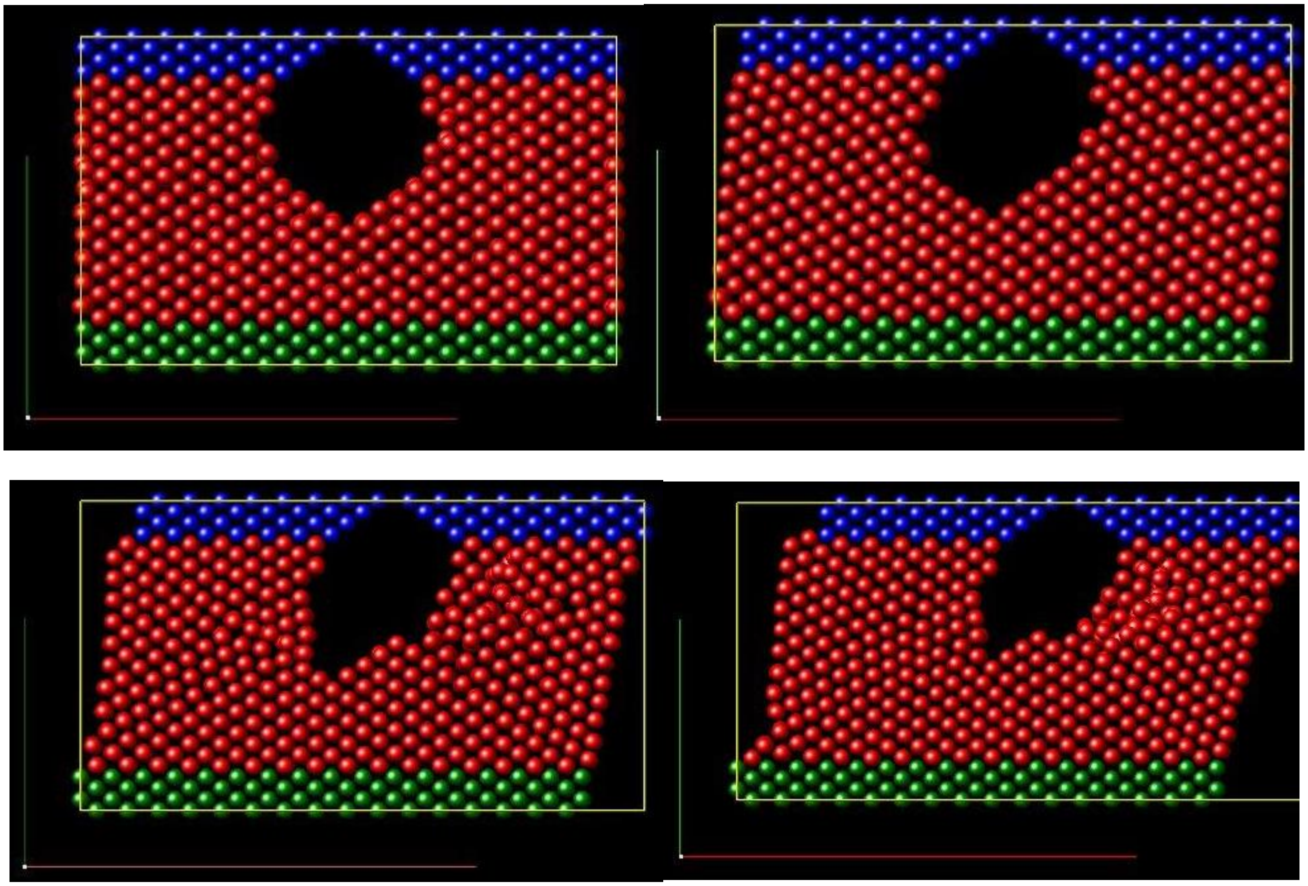


Fig 3.1: Simulations at time step 0, 1000, 2000, 3000

## 2. ***Tension Simulation of Copper upon application of Temperature Change:***

I. LAMMPS input script

  a) Initialization: 3-D simulation block of 10*10*10 is defined with periodic boundaries.

  b) Atom Definition: FCC lattice is defined.

  c) Force Fields: Cu.meam potential file is called to define the atoms. meam potential is used to define Copper atoms properties.

  d) Compute: Stress Null vector is created.

  e) Equilibration: Velocity is created to seed number 12345 at 300K randomly.

  f) Settings: Ensemble is fixed to npt at 300K temperature.

  g) Dump: The stress analysis is dumped in dump.Cu.equil* at a time step of 400 and run for 4000 simulations.

  h) Dump: The complete analysis is dumped in dump.Cu.tension.* at a time step of 400 and run for 4000 simulations.

II. The input script is run in command prompt in serial version which is side by side saved in a log.lammps file to be reviewed later

III. OVITO: The dump file is loaded in OVITO and the simulation is viewed with time.

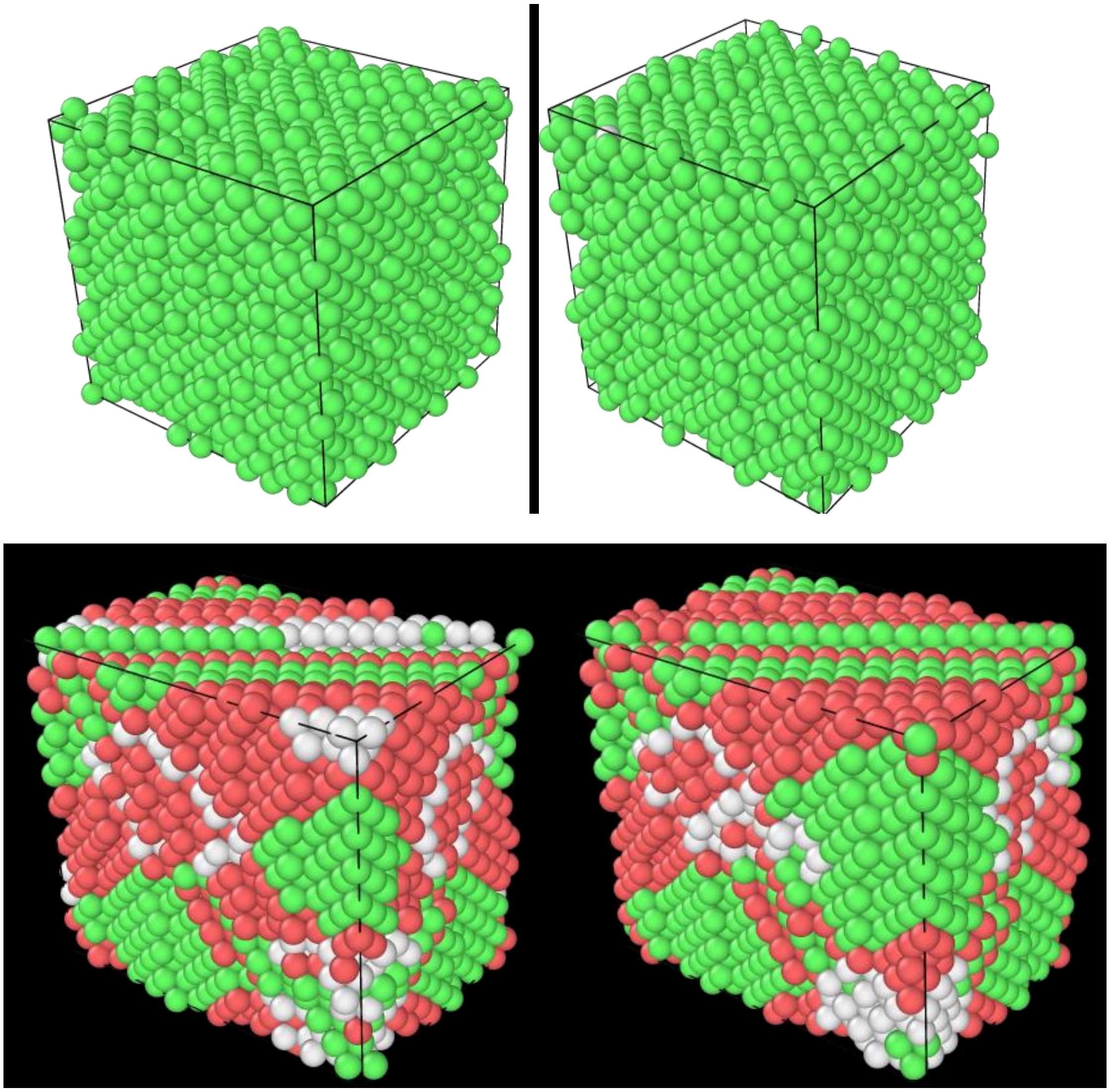


Fig 3.2: Simulations at time steps 0, 1250,2800,4000

## 3. *Compression Simulation of Copper upon application of Temperature Change: -*

I. LAMMPS input script

  a) Initialization: 3-D simulation block of 10*10*10 is defined with periodic boundaries.

  b) Atom Definition: FCC lattice is defined.

  c) Force Fields: Cu.meam potential file is called to define the atoms. meam potential is used to define Copper atoms properties.

  d) Compute: Stress Null vector is created.

  e) Equilibration: Velocity is created to seed number 12345 at 300K randomly.

  f) Settings: Ensemble is fixed to npt at 300K temperature.

  g) Dump: The stress analysis is dumped in dump.Cu.equil* at a time step of 400 and run for 4000 simulations.

  h) Dump: The complete analysis is dumped in dump.Cu.comp.* at a time step of 400 and run for 4000 simulations.

II. The input script is run in command prompt in serial version which is side by side saved in a log.lammps file to be reviewed later

III. OVITO: The dump file is loaded in OVITO and the simulation is viewed with time.

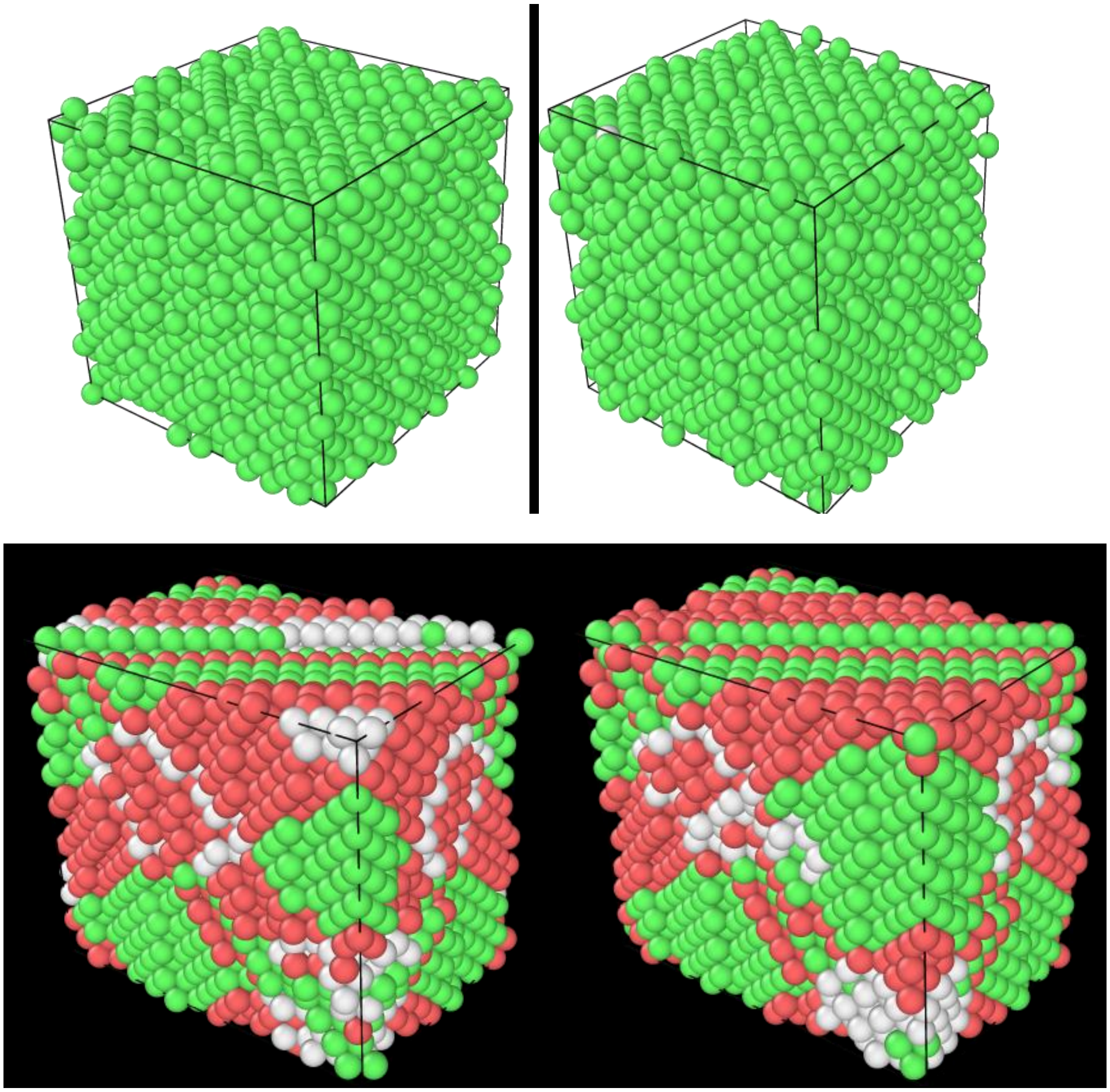


**Fig 3.3: Simulations at time steps 0, 1250,2800,4000**

## 4. ***Compression simulation of Copper and Aluminum Alloy upon application of Temperature Change: -***

I. LAMMPS input script

a) Initialization: 3-D simulation block of 10*10*10 is defined with periodic boundaries that contains 2 boxes.

b) Atom Definition: Simple Cubic lattice for both boxes as well as the complete Simulation. Copper atoms are created in box 1 and Aluminum atoms in box 2 whose origin is at (0.5,0.5,0.5)

c) Force Fields: meam potential is defined. AlCu.meam and library.meam fils are called to define the properties of Copper and Aluminum individually and as an alloy.

d) Equilibration: Velocity is created to seed number 12345 at 300K randomly and NPT ensemble is fixed.

e) Thermo Output Setting: Time step of 1000 is fixed and the simulation is run for 2000 steps.

f) Deformation: A compressive deformation is set in the x direction.

g) Variable v_strain is defined

h) Value of strain developed is printed in the log file.

i) Dump: The complete analysis is dumped in dump.two-element at a time step of 1000 and run for 20000 simulations.

II. The input script is run in command prompt in serial version which is side by side saved in a log.lammps file to be reviewed later

III. OVITO: The dump file is loaded in OVITO and the simulation is viewed with time.

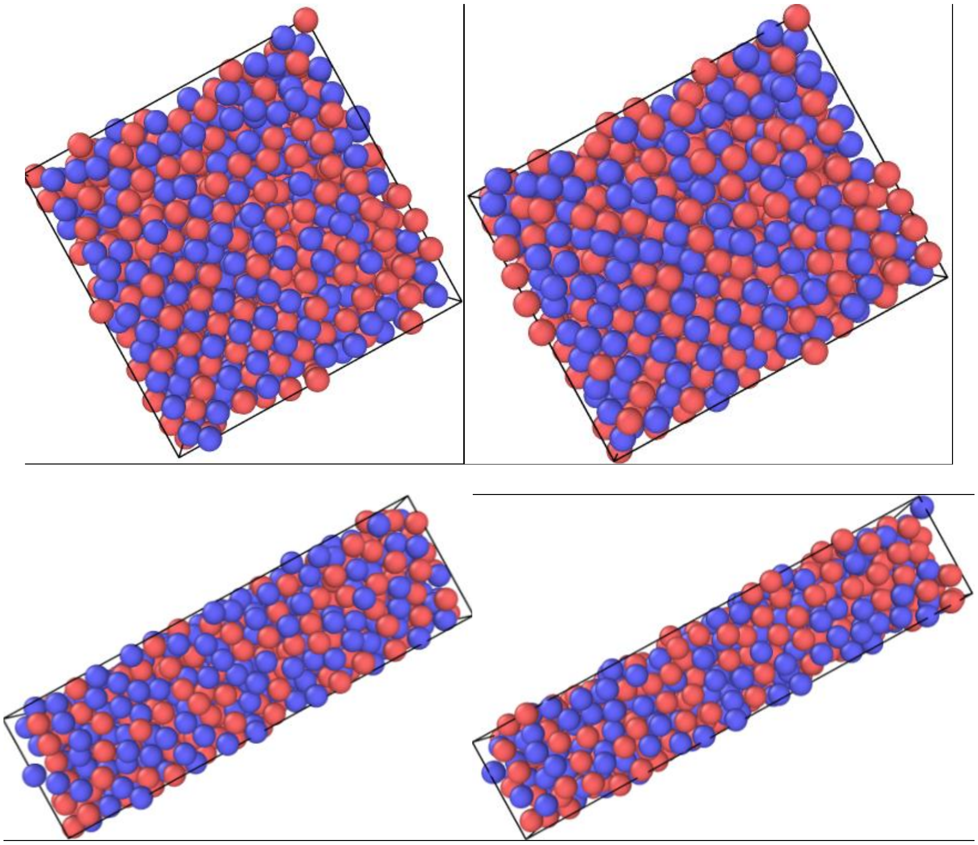


**Fig 3.4: Simulations at time steps 0, 1250,2800,4000**

## 5. ***Unidirectional Failure of pure elemental Iron under Tension: -***

I. LAMMPS input script

a) Initialization: 3-D simulation with periodic boundaries is defined.

b) Atom Definition: Data file of Iron in BCC crystal lattice created from material studio is called for the positions and determination of mass and volume.

c) Force Fields: eam/fs potential is used. Fe_mm.eam.fs file is called to determine interatomic properties of Fe.

d) Regions: The whole block is divided into 3 regions and grouped. Lower , Upper and Others.

e) Equilibration: timestep of 0.1 fs is taken. Using the berendsen thermostat temperature is fixed to 300K with damping factors of 100. NVE Ensemble is fixed. This part of the simulation is dumped in Equillibration.lammpstrj which contains runs of 1000000 times with a timestep of 1000.

f) Deformation: Deformation is applied to the block.

g) Settings: Ensemble is fixed to nvt at 300K temperature for Others group.

h) Compute: Stress Null vector created and magnitude formula of stress is defined.

i) Dump: The stress analysis is dumped in e1017.lammpstrj at a time step of 400 and run for 4000 simulations.

j) Dump: The complete analysis is dumped in final.lammpstrj at a time step of 1000 and run for 600000 simulations.

II. The input script is run in command prompt in serial version which is side by side saved in a log.lammps file to be reviewed later

III. OVITO: The dump file is loaded in OVITO and the simulation is viewed with time.

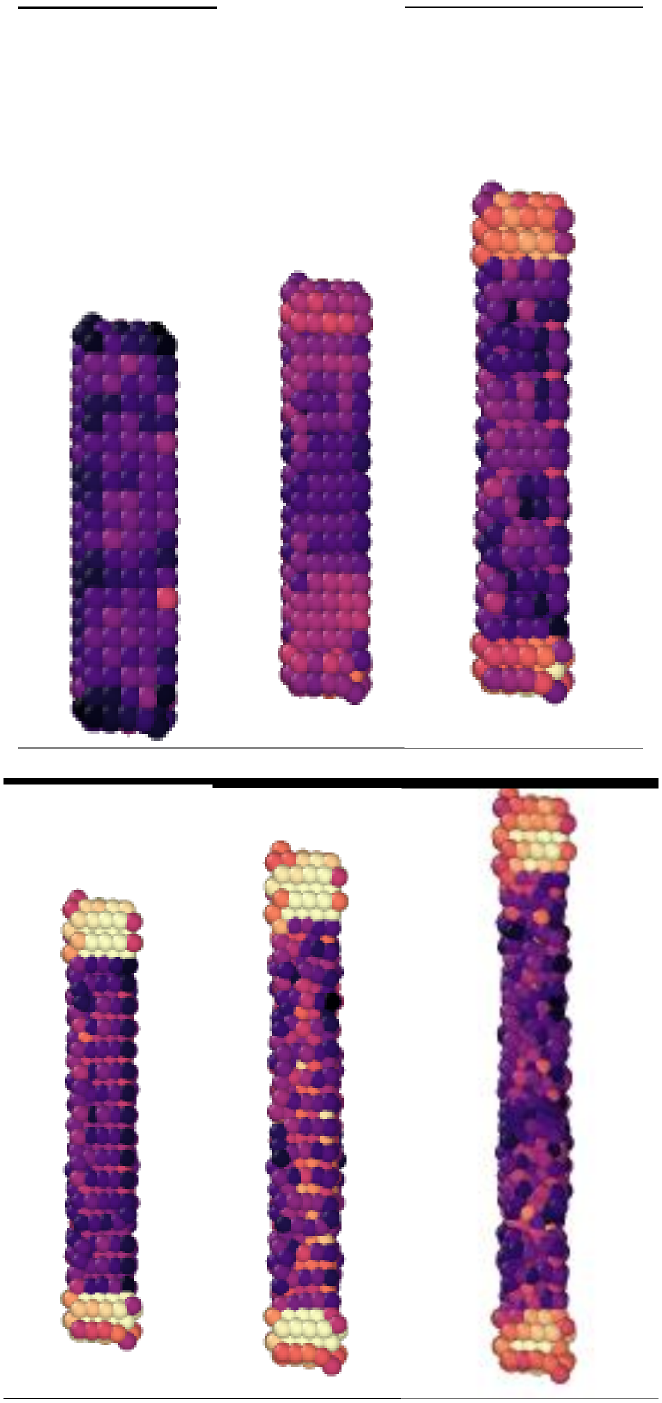


Fig 3.5: Simulations at time steps 0, 10000,80000,400000

## 6. ***CSH Gel Study:***

I. Calcium–silicate–hydrate (or C–S–H), an inosilicate, is the major binding phase in cement pastes and concretes and a porous hydrated material made up of a percolated and dense network of molecules of CSH gel arranged randomly.

II. Calcium– silicate–hydrate (or C–S–H with C = CaO; S = $SiO_2$; H=$H_2O$)

III. C–S–H nanoparticles nucleate and grow during cement hydration from a supersaturated solution produced by the dissolution of a cement clinker when mixed with water; for the most widely used formulations, the ratio of Ca to Si is ∼1.7.

IV. Mass of CSH gel varies according to requirements and clinker compositions. Approximate Mass of CSH Gel = 1063kg/mol

V. Modulus of Elasticity is generally between 15 - 30 Gpa

VI. Density~1.8 to 2.1

VII. LJ parameters for CSH gel $\varepsilon_{ij}$ = 140 kJ/mol, $\sigma_{ij}$= 2.02 [nm]

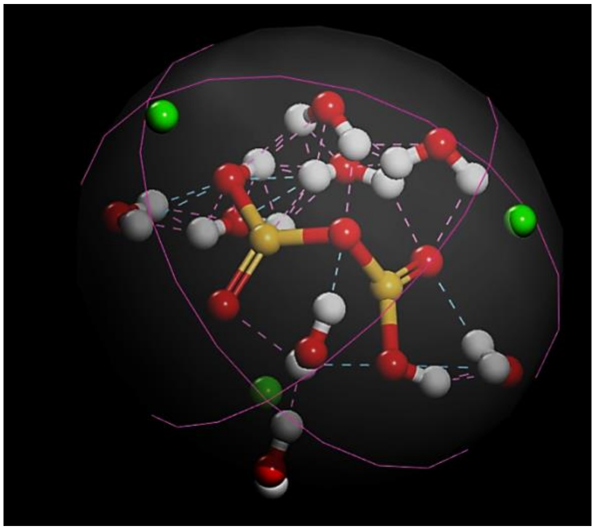


Fig 3.6: CSH gel individual Molecule structure modelled in Material Studio

## 7. *Simulation of CSH Gel: -*

I. LAMMPS input script

a) Initialization: units are set to real, and periodic boundaries in all 3 dimensions.

b) Atom Definition: A 100*100*100 cubic units simulation box is created with 1200 molecules of 1091 mass are *placed randomly*.

c) Force Fields: LJ potential is defined with cutoff radius set to 25 Angstroms and LJ potential parameters defined as $\varepsilon_{ij}$ = 8420 kCal/mol and $\sigma_{ij}$= 20.2 A.

d) Groups: Lower, upper and mobile regions are defined and grouped.

e) Minimization: Since randomization is used to avoid overlapping and loss of atoms during simulation energy is minimized using minimize command with a timestep of 1000.

f) Equilibration and Fixes: NVE ensemble is defined at a temperature of 270 K. Lower region group atoms are fixed by setting a force of 0 units on them.

g) Deformation: A deformation in the form of a strain of 0.02 is applied on all the atoms

h) Compute: Stress Null vector is created and magnitude of average stress in one directional is defined and dumped to a file named e1017.lammpstrj with a timestep of 1000 each being of 3 ps.

i) Dump: The complete analysis is dumped in crack.dump at a time step of 1000 and run for 15000 simulations. Also, a movie of the simulation is dumped and also the individual images of the simulation at each time step.

II. The input script is run in command prompt in serial version which is side by side saved in a log.lammps file to be reviewed later

III. OVITO: The dump file is loaded in OVITO and the simulation is viewed with time.

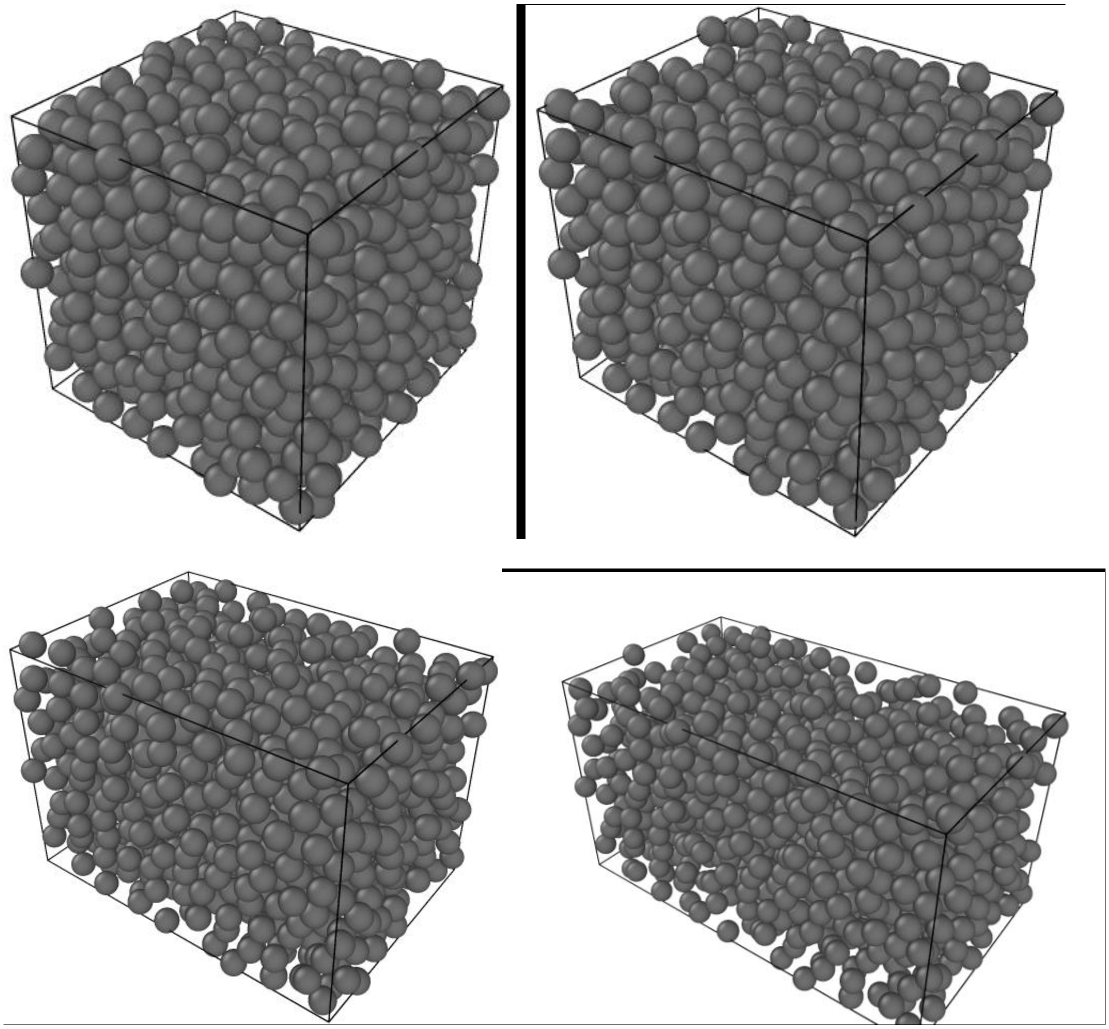
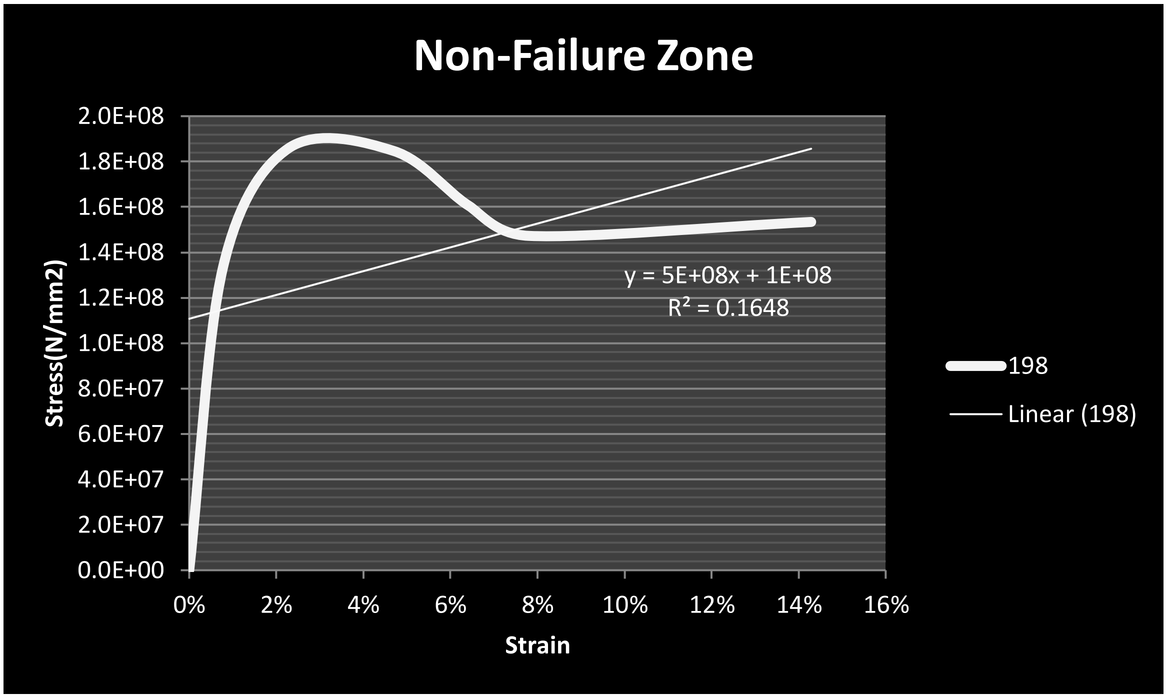


Fig 3.7: Simulations at time steps 0, 2, 6,10

## 8. ***Analysis of CSH Gel: -***

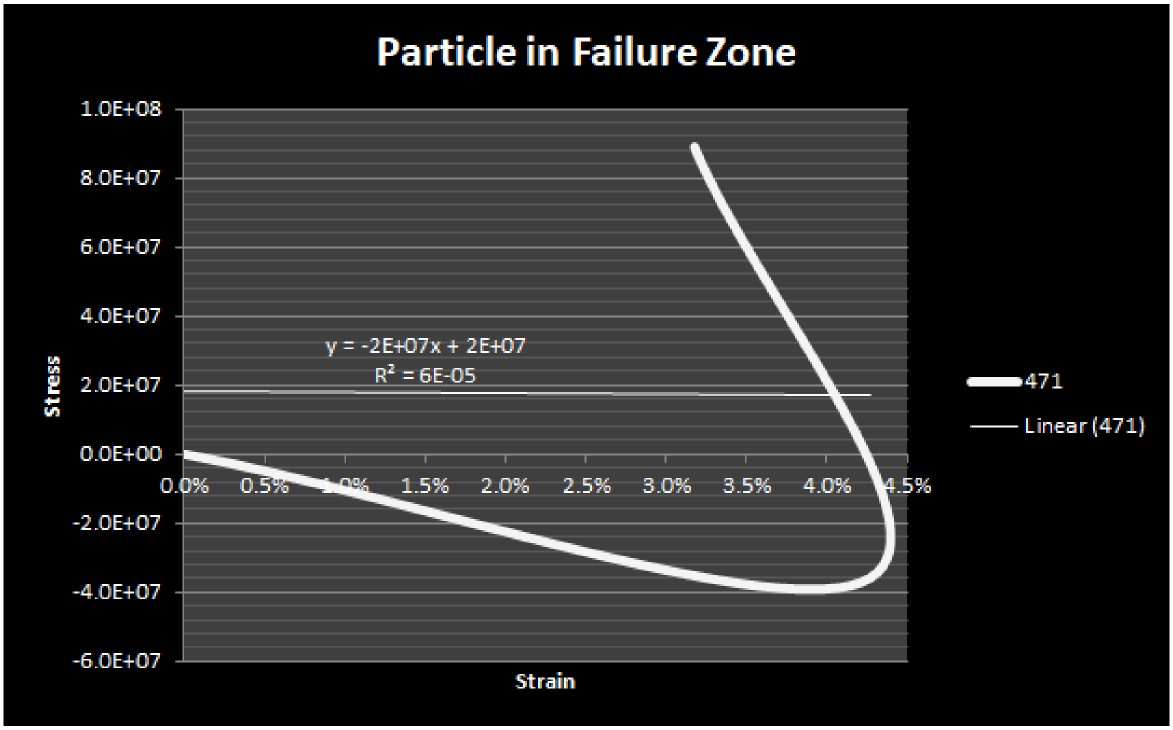
I. Particles are randomly chosen at different positions of the simulation box.

a) Particle 198 is almost in the middle of the simulation box, away from the failure zone.

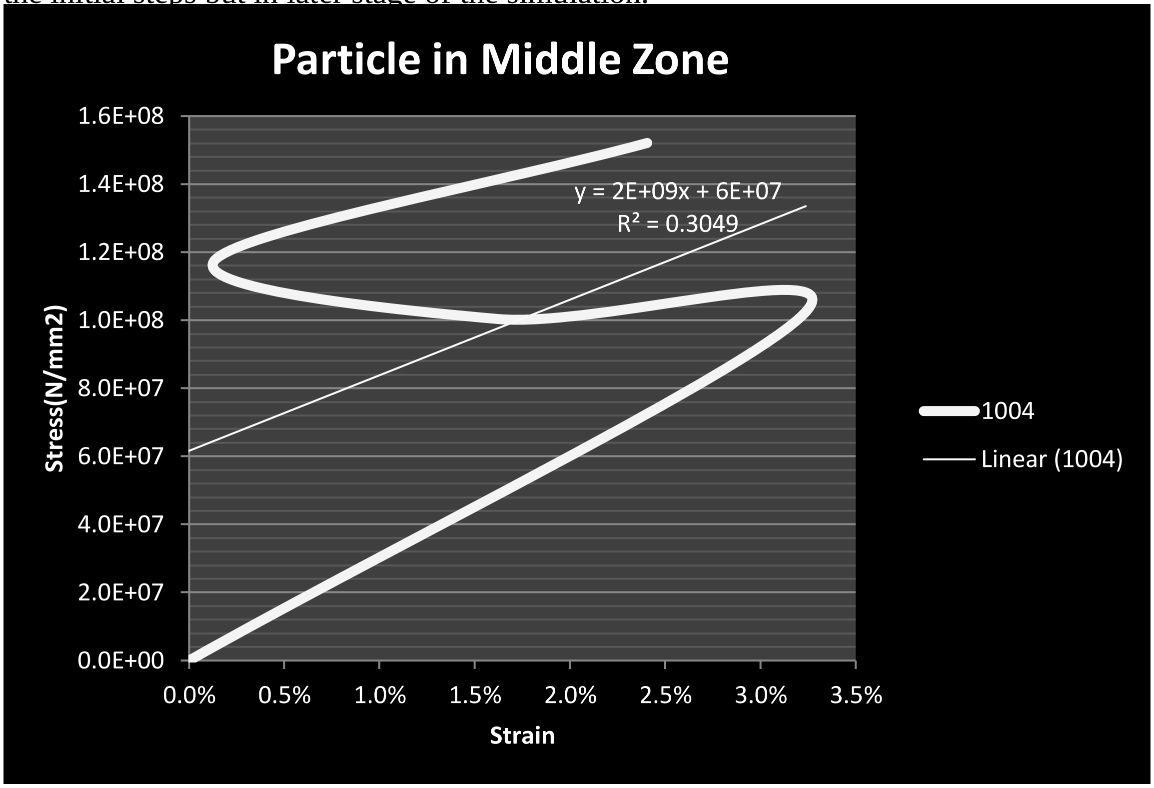


i. Young's Modulus E = 17.1 Gpa

b) Particle 471 lies in the failure zone. Hence graph is unpredictable

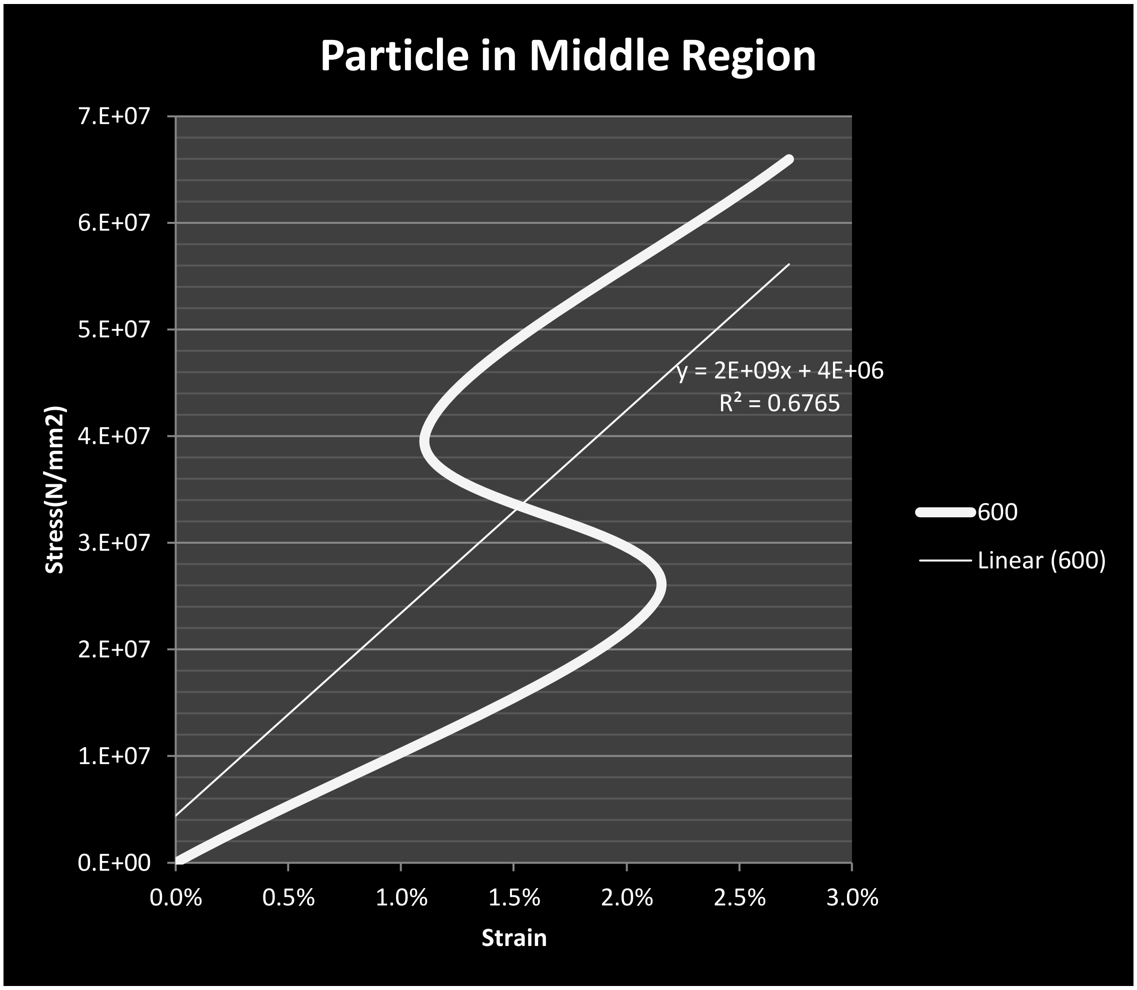


c) Particles in the region adjacent to the failure region and the middle that do not fail in the initial steps but in later stage of the simulation.



i. Young’s Modulus = 6.17Gpa

d)



i. E = 3.63 GPa

II. Mean Value of E = 9 Gpa

## 9. ***Study of Concrete: -***

I. Concrete consists of 60 percent of CSH gel- acts as binding material.

II. Density: 2.4 kg/$m^3$

III. Weaker in Tension

IV. Concrete is a random arrangement of CSH gel molecules and different Aggregates.

V. Mass variable

VI. Here, Quartz is taken as the aggregate whose density is approximately 2.67

VII. LJ parameters approximated: -

  a) LJ parameters of CSH gel are known

  b) LJ parameters of Quartz –Quartz and CSH Quartz not known

  c) Since Quartz-Quartz interactions are weaker, a low value of sigma and epsilon in comparison to CSH gel interactions are considered.

  d) CSH- Quartz interactions are calculated as: -

    i. Sigma equals the arithmetic mean of CSH-CSH and Quartz-Quartz sigma values

    ii. Epsilon equals the geometric mean of CSH-CSH and Quartz- Quartz epsilon values.

  e) Hybrid characteristics of LJ potential in LAMMPS help incorporate the 3 different potentials.

---

## 10. ***Simulation of Concrete: -***

I. LAMMPS input script

a) Initialization: units are set to real, and periodic boundaries in all 3 dimensions.

b) Atom Definition: A 100*100*100 cubic units simulation box is created with 1200 molecules of 1091g/mol mass and 1000 atoms of 120 g/mol mass are *placed randomly*.

c) Force Fields: LJ potential is defined with cutoff radius set to 25 Angstroms and LJ potential parameters defined as $\varepsilon_{ij}$ = 8420 kCal/mol and $\sigma_{ij}$= 20.2 A.

d) Groups: Lower, upper and mobile regions are defined and grouped.

e) Minimization: Since randomization is used to avoid overlapping and loss of atoms during simulation energy is minimized using minimize command with a timestep of 1000.

f) Equilibration and Fixes: NVE ensemble is defined at a temperature of 270 K. Lower region group atoms are fixed by setting a force of 0 units on them.

g) Deformation: A deformation in the form of a strain of 0.02 is applied on all the atoms

h) Compute: Stress Null vector is created and magnitude of average stress in one directional is defined and dumped to a file named e1017.lammpstrj with a timestep of 1000 each being of 3 ps.

i) Dump: The complete analysis is dumped in crack.dump at a time step of 1000 and run for 15000 simulations. Also, a movie of the simulation is dumped and also the individual images of the simulation at each time step.

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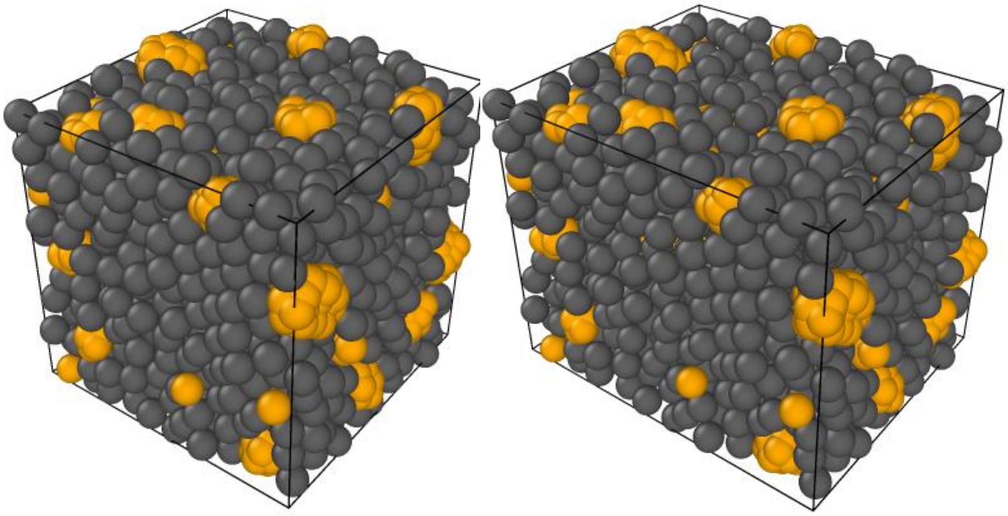


Fig 3.11: OVITO rendered images of Initial and Final Condition of Structure

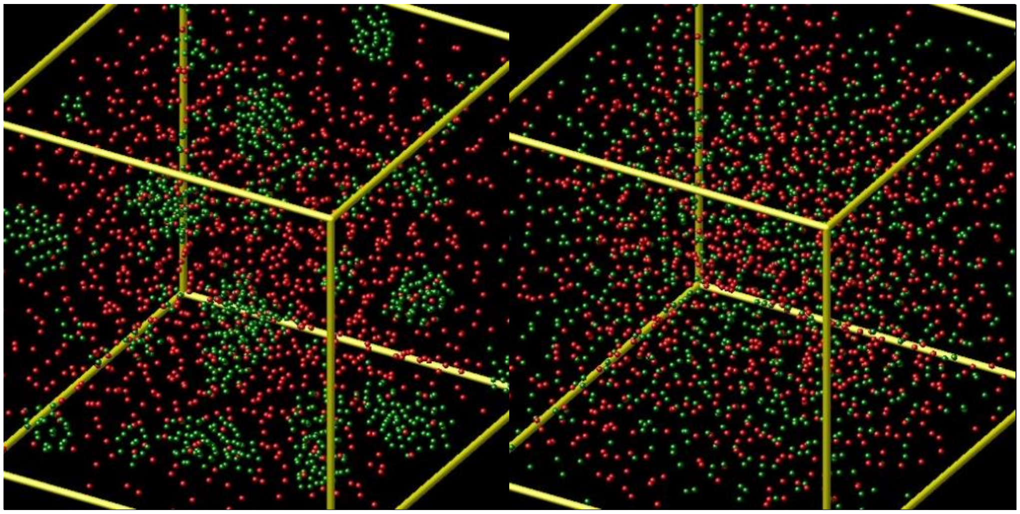
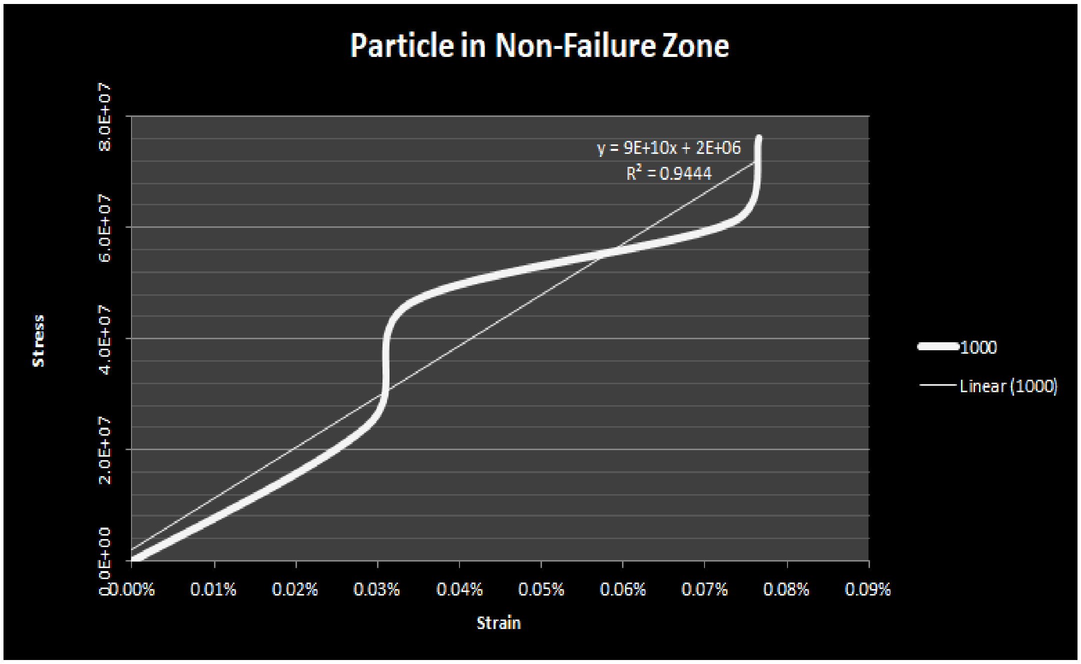


Fig 3.12: LAMMPS dumped images of initial position and final position of molecules

## 11. *Analysis of Concrete Simulation:*

I. 3 molecules are considered from the simulations and analyzed. These molecules, since randomly arranged are in different parts of the simulation box.

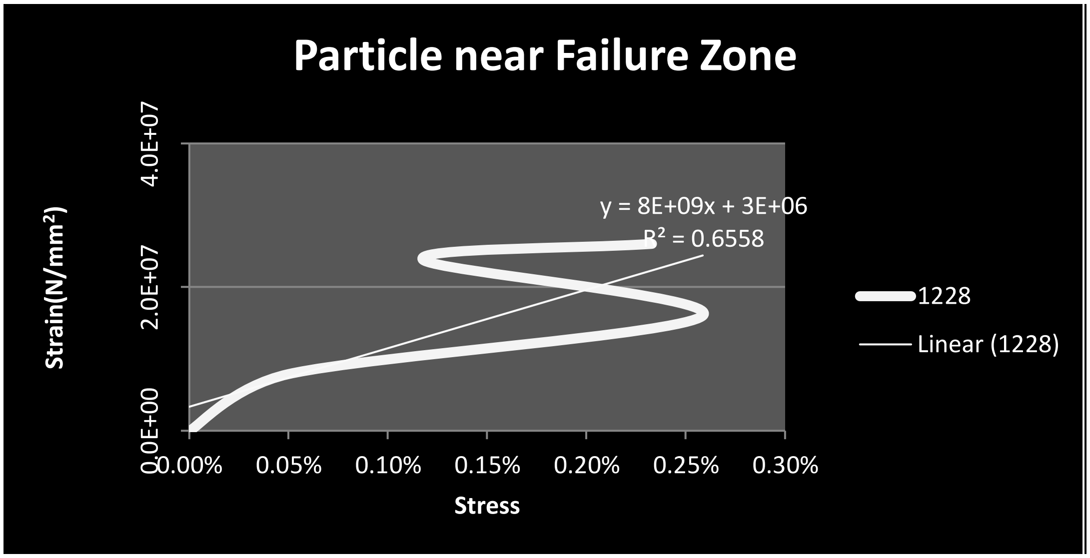
a) Away from the failure region in the middle region of the simulation box.



i. E = 80 GPa

ii. Failure Stress = 61 Mpa

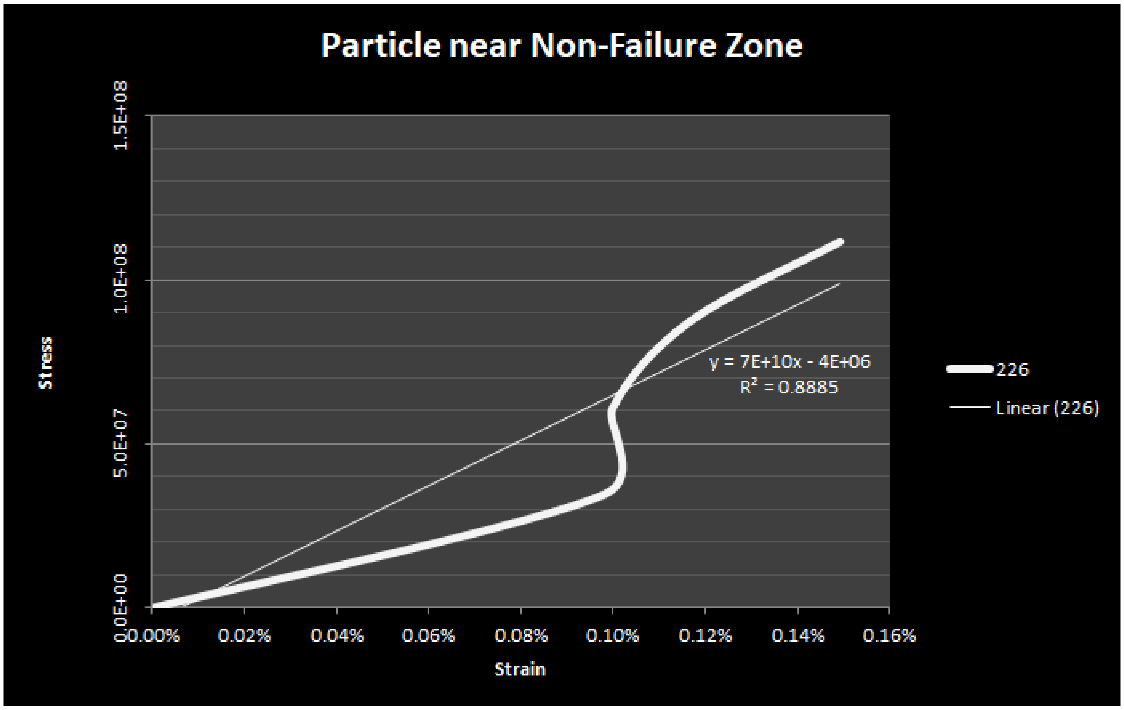
b) In the failure region



i. E = 20 GPa

ii. Failure Stress = 16 Mpa

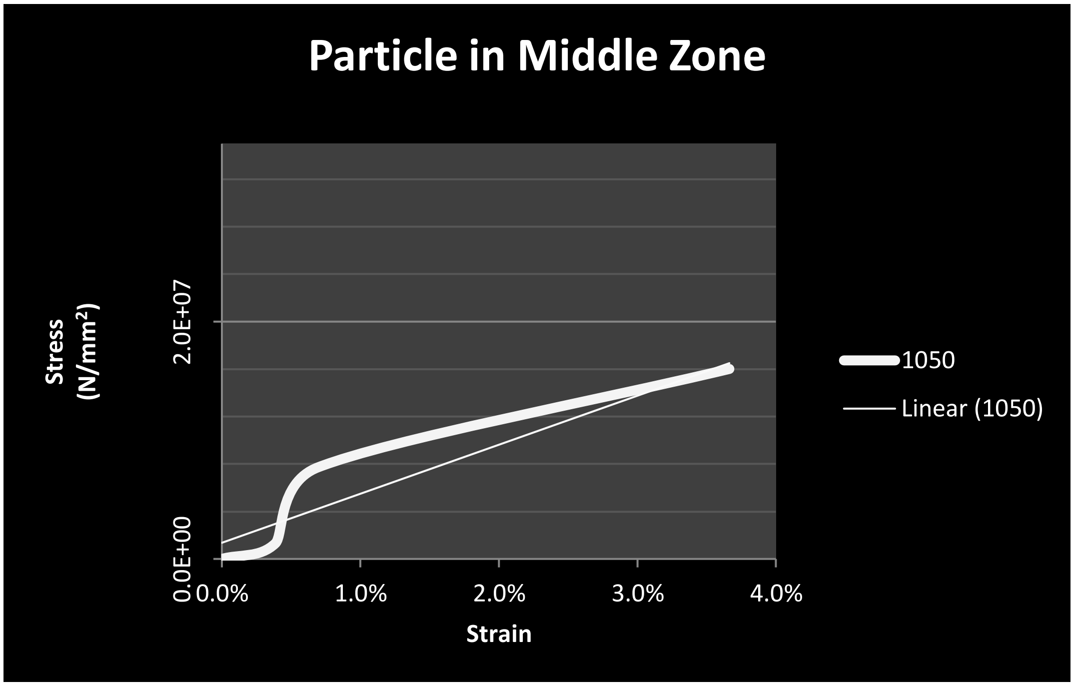
c) Between the failure region and center:



i. E = 35.27 GPa

ii. Maximum Stress = 60.7 Mpa

d)



i. E = 4 Gpa

ii. Maximum stress = 16 Mpa

II. Mean value of E = 34.82 GPa

III. Mean of Max Stress = 38.425 Mpa

# Chapter 4: Conclusion and Future Scope

## 4.1. Conclusion:

The best possible way to analyze a structure is by understanding and visualizing it in depth. Visualization at atomic and molecular level is one of the best methods to analyze the structure. Molecular Dynamics helps one create, visualize and analyze structures at nanoscale giving an insight to what must be happening. In this project, analyzing pure atom structures and different combined molecular structures is a step by step procedure. The following points are concluded: -

- The simulation for CSH has helped us come to the conclusion that the Young's Modulus Values occurring during the simulation are lesser than but in comparative scale to the experimentally observed values. As the properties vary according to the presence of different amount of clinkers and water, difference in values are justified. Also, voids and other impurities aren't taken into account which is making the CSH gel weaker here.
- Concrete Simulations have both young's modulus and failure stresses in almost the range of experimentally observed values. As defects are not considered, the strength values are comparatively in the higher range of experimentally observed values.
- The results conclude that the method of molecular dynamics simulation using Vander Waals Potential interaction between atoms and molecules under physical conditions give accurate results.

4.2. **Future Scope:** The developed randomized structure of Cement and Concrete along with the following method could be used in further research as well. With proper conditions given, they can be used to eliminate experiments in most cases. The time consumption of days could be reduced to hours and even to minutes if multiple processors are used. Also density variations, temperature variations, their effects and even reinforcement predictions to much more accuracy can be done in the coming times.

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# Publication

Namrata Singh, Saikat Sarkar,” Randomized Model of Cement and Concrete”, *to be submitted in an International Journal*.

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