

MOLECULAR DYNAMICS SIMULATION OF NANOINDENTATION TEST OF  
CORUNDUM ( $\alpha$ -Al<sub>2</sub>O<sub>3</sub>) ON (0001) SURFACE

By

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## LIST OF ABBREVIATIONS

HCP	hexagonal close-packed
HPC	High Performance Computer
MD	molecular dynamics
PBC	periodic boundary conditions
VMD	Visual Molecular Dynamics

Abstract of Thesis Presented to the Graduate School  
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Requirements for the Degree of Master of Science

MOLECULAR DYNAMICS SIMULATION OF NANOINDENTATION TEST OF  
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Major: Mechanical Engineering

Corundum ( $\text{Al}_2\text{O}_3$ ) is a material with high hardness. So it is widely used in making cutting tools and armors. Lots of experiment tests have been made to evaluate its properties and find some atomic reaction during the loading.

Molecular dynamics (MD) simulation is a powerful tool to study the material in atomic scale. Due to its feature of reproducible and high efficiency, MD is becoming a preference for more and more researchers whose field is related to nanotechnology. With the improvement of computer hardware performance, this tool is turning much stronger than before.

This thesis aims to see the atomic behavior of corundum ( $\text{Al}_2\text{O}_3$ ) under nanoindentation loading, which is a very popular way in experiment to measure the mechanical properties and get the atomic structure changes, on (0001) surface of  $\alpha$ - $\text{Al}_2\text{O}_3$  using MD simulation software LAMMPS.

MD simulation method, which is with the advantages of reproducible and low-costing, is fast developing in the past decade along with the significant improvement of computer power.

Indentation test is a good way to measure the properties of hardness material. The MD indentation simulation for  $\text{Al}_2\text{O}_3$ , can let us know the behavior when the material under a certain loading. And the strain rate, temperature and specimen size effect analysis can help us to figure out a proper way to do the simulation for this material.

## CHAPTER 1 INTRODUCTION

### **Motivation**

Super hard materials has widely put into use in many fields, including being used as the main component of personnel armor, cutting and polishing tools and anti-wear coating. Study on the material exists in natural world can help us know why it has that property and give us hints and ideas to design new material. [1]

Since corundum has a very good mechanical reaction behavior during the loading. And MD simulation is a good tool to do this kind of study. While for many reasons, few research on the mechanical properties of  $\text{Al}_2\text{O}_3$  using the MD simulation method found. Therefore, this study is going to do some attempts on the study for corundum under a mechanical loading with MD simulation software LAMMPS.

### **Corundum**

Corundum ( $\text{Al}_2\text{O}_3$ ) is a kind of super hard material, so it is widely used for ballistic protection. And it is also one of the most important ceramic materials today. Lots kind of armors, such as ALOTEC 96 SB, ALOTEC 98 SB, ALOTEC 99 SB and ALOCOR 100, are mainly consist of  $\text{Al}_2\text{O}_3$ .

Corundum, whose chemical formula is  $\text{Al}_2\text{O}_3$ , is the third hardest natural mineral known to science. As we all known, diamond is the hardest mineral, and four times harder than corundum. The second hardest is Moissanite (Silicon Carbide) at 9.25 barely beats corundum's hardness of 9.0.

Corundum is a crystalline of aluminum oxide ( $\text{Al}_2\text{O}_3$ ). Commonly, natural-exist corundum is called by ruby (red) or sapphire (any color except red). Because of the beautiful color and appearance, ruby and sapphire are considered as gem for

ornamental uses. [2]  $\text{Al}_2\text{O}_3$  has a lot of phases including  $\gamma$ ,  $\kappa$  and  $\eta$  phases. [3] Phase transition or amorphization maybe happen under some conditions. Among all of polymorphic phases,  $\alpha\text{-Al}_2\text{O}_3$  is the most stable one. Table1-1 shows the general information and mechanical constants of corundum. [2]

Table1-2 shows the Mohs hardness levels and the absolute values. [4] The hardness of corundum is 4 times bigger than the quartz ( $\text{SiO}_2$ ), which is think is hard enough commonly. In some extent, the strong and short oxygen-aluminum bonds contribute the hardness of corundum. The oxygen and aluminum atoms were pulled close together by those bonds. Note that the bonds make the crystal not only hard but also quite dense for a mineral made up of two relatively light elements. Due to its high melting point and high hardness, corundum is considered as a kind of ceramic armor and has become a dominant one at the armor material market.

## **Molecular Dynamics Simulation**

### **Principals of MD**

How the computational materials approach utilizes different time and length scale analysis methods, as illustrated in Figure 1-1. [5] As we all known, atoms are the building blocks of all materials. And the length interatomic distance, which is mostly the length of the bonds of atoms, is measured by the unit called angstrom ( $\text{\AA}$ ), which is equal to  $10^{-10}$  m (one ten-billionth of a meter).

MD simulation is an effective tool to study the material in Nano-scale. Just like FEA, the simulation tool which has been widely used in Engineering Field. FEA Simulation software tool can give us the result of a structure under a certain loading. We just need to do the modeling of a structure, input some material constants and give it a

load. MD is kind of a way like FEA. The difference is that the time and length scale. For MD, the length and time scale are  $10^{-10}$  m and  $10^{-12}$  s.

Figure 1-2 shows the overview of MD. In the middle of the figure is MD simulator. The left side is the input of MD and the right side is the output of MD. In this figure, we can get what are needed if we want to do a MD simulation. For this research the MD simulator I used is LAMMPS. In this software all of them can be inputted by the LAMMPS commands. Sometimes some other tools are also necessary, such as some the potential or some initial position of atoms is needed to programming. Just like the model of this study is established by the FORTAN programmer.

At the right side of the figure, there are the outputs we can get from MD simulation. Actually, trajectory is the only output directly from MD simulator, and other values including forces, energy of the system, temperature, pressure and so on are come from the trajectories. These values are significant to do analysis.

In the most common version, the trajectories of atoms and molecules are determined by numerically solving the Newton's equations of motion (Eq. 1-1) for a system of interacting particles, where forces between the particles and potential energy are defined by molecular mechanics force fields. That is why we need a potential. In other words, the potential gives the rule that what reaction the atom should have under a certain force, and either the force resulted the movement of an atom.

$$F = ma = m \frac{dv}{dt} = m \frac{d^2r}{dt^2} \quad (1-1)$$

The resultant force  $F$  can be obtained from potential energy  $U(r)$ , which is a function of atomic positions.

$$F = -\frac{\partial U(r)}{\partial r} \quad (1-2)$$

## **Periodic Boundary Conditions**

In MD simulation research, the scale of the model will affect the simulation running results. One of the reasons is the boundary effect. Of course, a large model with more particles can be implemented, but that will lead to a significant increase in runtime. As we know, MD simulation has a limitation that it cannot hold the specimen as big as the experiment test because of the limited and insufficient computer power. To reduce the boundary effect without high cost on improving the computer power, MD simulation offers a way to simulate a large system by modeling a small part that is far from its edge. That approach is called periodic boundary conditions (PBC).

Periodic boundary conditions can be used in each dimension of Cartesian coordinates (e.g. x or y or z). When applying two dimensions with PBC, we call it slab boundary conditions. [6] This is the condition I am going to use in this research.

The Figure 1-3 is aiming to tell you schematically. It is a 2D figure. The red rectangle represents the real model we have in the simulation. And the white ones are the copy of the red one. Once the PBC are adopted, two results we will have: one is that the atom leaves from one boundary of the simulation box will appear in the opposite side of the box instantly with the same velocity. The other is that, the behavior of the atom near one face of the simulation box will be interacted by the ones at the other side of the box.

## **Time Integration Algorithms**

Due to the complex nature of potential energy functions, there is no analytical solution to the integration of Newton's equation. Thus, time integration algorithms are used.

Time integration algorithm is most critical part of MD simulation code. So lots of people call it to be “the engine of MD program”. Finite difference algorithm does the integration of the equations of motion for the interacting atoms. Then the forces can be computed and the location of the atoms can be tracked.

Among many time integration methods for the molecular dynamics simulation, Verlet and predictor-corrector are the two most accepted by people. Meanwhile, we have to admit that these kinds of methods are all based on some approximation, which is neglecting the higher order of Taylor expansion. So the accuracy will be reduced by that. The main inaccuracy is come from truncation errors and round-off errors. But we should note that, the smaller time step can minimize those errors. But simultaneously, that would lead the calculation time increasing. [7]

“Predictor-corrector methods advance the simulation in time by predicting an acceleration with a Taylor expansion then later correcting the acceleration when the force is formally evaluated from the gradient of the potential. These methods require eight arrays of size  $3N$ , which is five more than required by the popular Verlet schemes. A specific interpretation is the Gear predictor-corrector, which is fifth order accurate and can use a longer time step than Verlet methods, thus making it both more accurate and more stable.

The Verlet algorithm is a good compromise between accuracy and performance. The MD algorithm in this thesis uses a Verlet variant known as the velocity Verlet algorithm which explicitly includes the velocity in the algorithm and is therefore self-starting when provided positions and velocities. Although it is mathematically identical to the standard Verlet scheme, the kinetic energy in the Verlet velocity algorithm may be

computed immediately rather than requiring an extra step to compute atomic velocities.”  
[7]

The time integration algorithm used in this research is called velocity verlet algorithm

$$r_i(t + \Delta t) = r_i(t) + v_i(t)\Delta t + \frac{F_i(t)}{2m}\Delta t^2 \quad (1-3)$$

$$v_i(t + \Delta t) = v_i(t) + \frac{F_i(t + \Delta t) + F_i(t)}{2m}\Delta t \quad (1-4)$$

### Radial Distribution Function

Radial distribution function is a statistical mechanics definition. To describe how density varies as a function of distance from a reference particle. [8] It is a measure of the probability of finding a particle at a distance of  $r$  away from a given reference particle.

The Figure 1-4 schematically illustrates what the RDF is. The red particle is our reference particle, and blue particles are those which are within the circular shell, dotted in orange. [8]

$$\rho = N/V \quad (1-5)$$

$$g(r) = 4\pi r^2 \rho dr \quad (1-6)$$

In Eq. 1-5,  $N$  is the number of blue particles;  $V$  is the volume of the space to be studied. For the RDF curve, the horizontal axis is  $r$  which is the distance from the reference particle. The vertical axis is  $g(r)$  the value of radial distribution function. Eq. 1-6 represents the relation of radial distribution function formula.

For a certain material which has an atomic structure, the RDF curve is corresponding to the atomic structure. That means the RDF curve variation can reflect

the change of atomic structure of a material. That is why we can use to analysis the phase transformation and amorphization of a material.

## **Software Tools**

### **LAMMPS**

LAMMPS, which is an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator, is open source classical molecular dynamics code. It is created and being maintained by Sandia National Laboratories, which is one of the laboratories of DOE. LAMMPS is a powerful software which has the ability to do the simulation of different kinds of materials including the biomaterials, which have a very complicated structure, and the traditional materials like metals and ceramics. In this case, it's potential for solid-state material is used since  $\text{Al}_2\text{O}_3$  is a kind of ceramics material.

The MD simulation needs large quantity of calculations. Larger number of atoms will leads longer calculation time.

Since the techniques are used to modify the running in parallel, LAMMPS has a great efficiency improvement when running on the parallel computer or workstation. Thereby, the number of calculation units decides the time using during the simulation progress. To reduce the running time, the high performance computer (HPC) in University of Florida is adopted instead of our single processor personal computer. Because the MD simulation is almost fully rely on the computer power, so the research related to MD is growing up along the significant improvement of computer power since 1990s.

When running in parallel, a technique called spatial-decomposition is applied to divide the whole domain of simulation into several 3D small boxes and align them to processors available. Each processor takes in charge of one box.

## Visual Molecular Dynamics

During the simulation progress, we can get lots of data including the force and displacement from the output files. Then we can get the load-displacement curve through Matlab or MS-Excel software. Meanwhile, for MD simulation, the data analysis is not enough. Since we need to know what happens when the force-displacement curve has an obvious trend change. For example, the displacement and phase transformation mostly happen when the curve has a drop. So, the visualization of what the atoms and the molecular model look like is significant important for this research case.

Currently, there are lots of codes or software available for visualization analysis. Among them, VMD is the most popular one and widely used for MD simulation. VMD is developed by a research group of University of Illinois at Champaign. Like LAMMPS, it is also open source. VMD can use the “.xyz” format file which can be outputted by LAMMPS. This file stores the total atom number for a certain model system and records the coordinate information of all atoms along the time changes.

By using the atom location information to animate what the real model looks like. VMD makes it possible to see the shape change and some microcosmic phenomenon. Research through experiment is always suffering from the difficulty to have a clear observation on the atomic scale. VMD deal with this problem and let us find the molecular structure change easily.

VMD offers a large color library for atoms and visualization styles. It supports the operation using either graphical interface or command lines. Figure 1-5 shows what the VMD windows look like.

Table 1-1. Properties of corundum

Property	Value
Chemical Formula	Al <sub>2</sub> O <sub>3</sub>
Density	4 - 4.1g/cm <sup>3</sup> , Average = 4.05 g/cm <sup>3</sup>
Melting point	2044C
Mohs scale hardness	9-Corundum
Crystal System	Trigonal ( $\bar{3}2/m$ )
Lattice constants	a=4.75 c=12.982 Z=6

Table 1-2. Mohs hardness levels and the absolute values

Mohs hardness	Mineral	Absolute hardness/ Gpa
1	Talc	1
2	Gypsum	3
3	Calcite	9
4	Fluorite	21
5	Apatite	48
6	Orthoclase Feldspar	72
7	Quartz	100
8	Topaz	200
9	Corundum	400
10	Diamond	1600

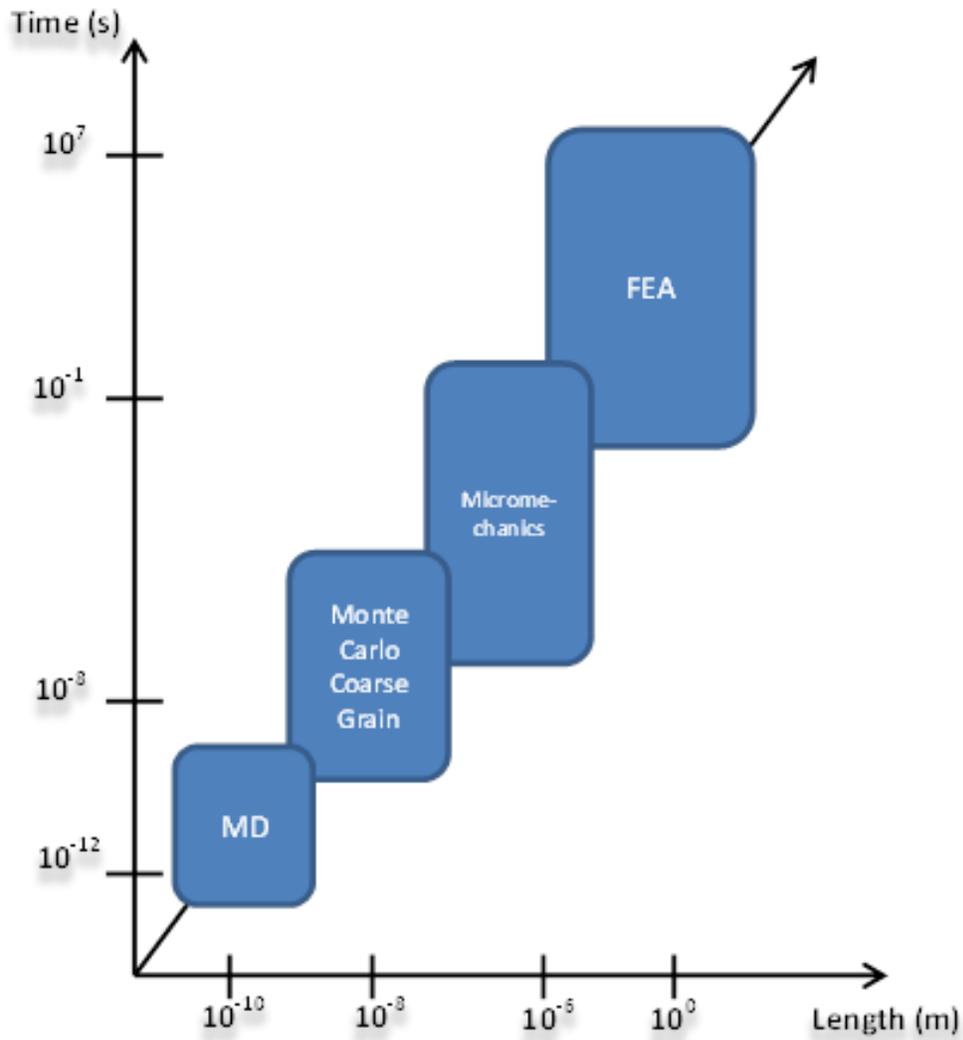


Figure 1-1. Modeling methods in discrete and continuum regions

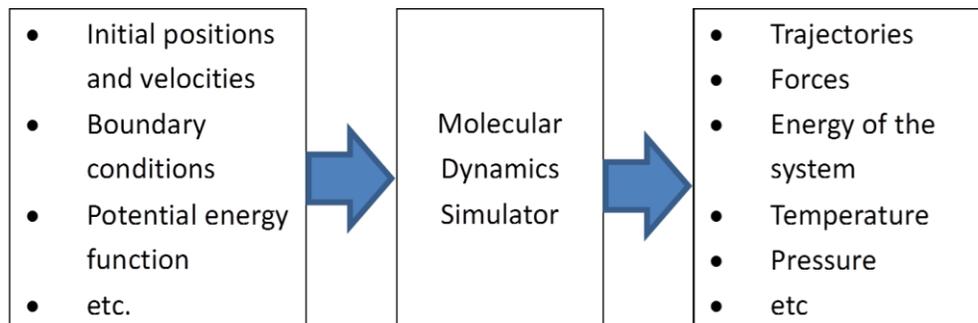


Figure 1-2. General view of MD simulation

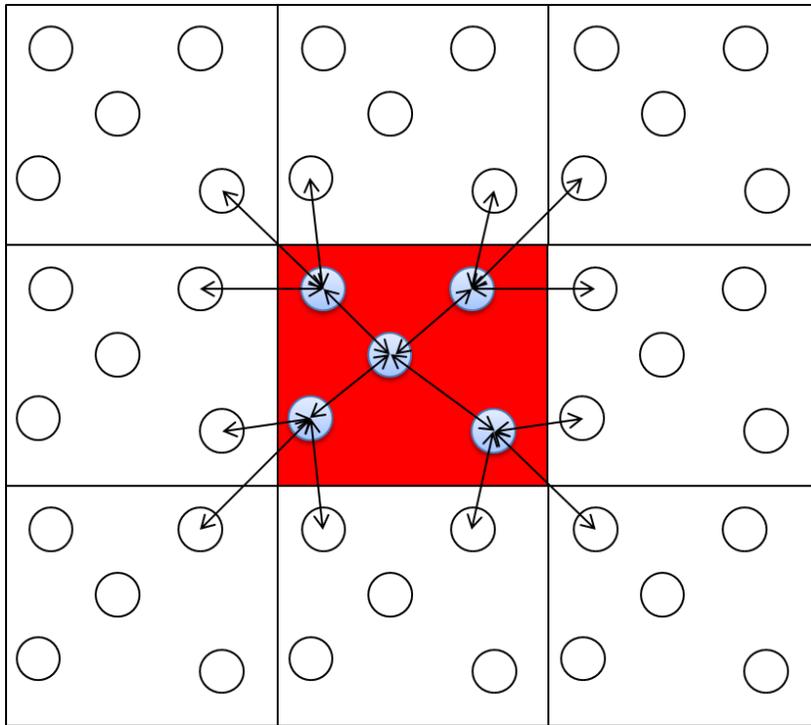


Figure 1-3. Periodic Boundary Conditions

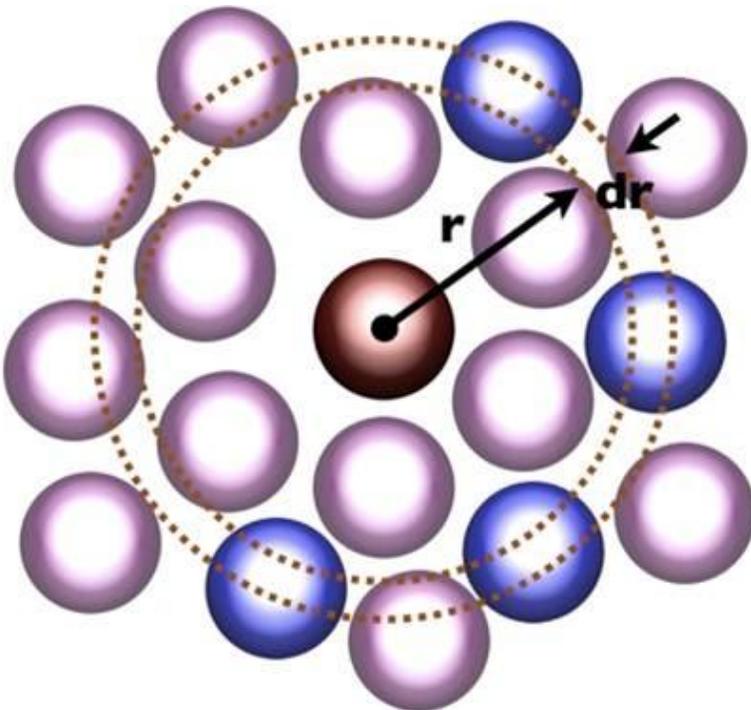


Figure 1-4. Radial distribution function (Source: [http://en.wikipedia.org/wiki/File:Rdf\\_schematic.jpg](http://en.wikipedia.org/wiki/File:Rdf_schematic.jpg)).

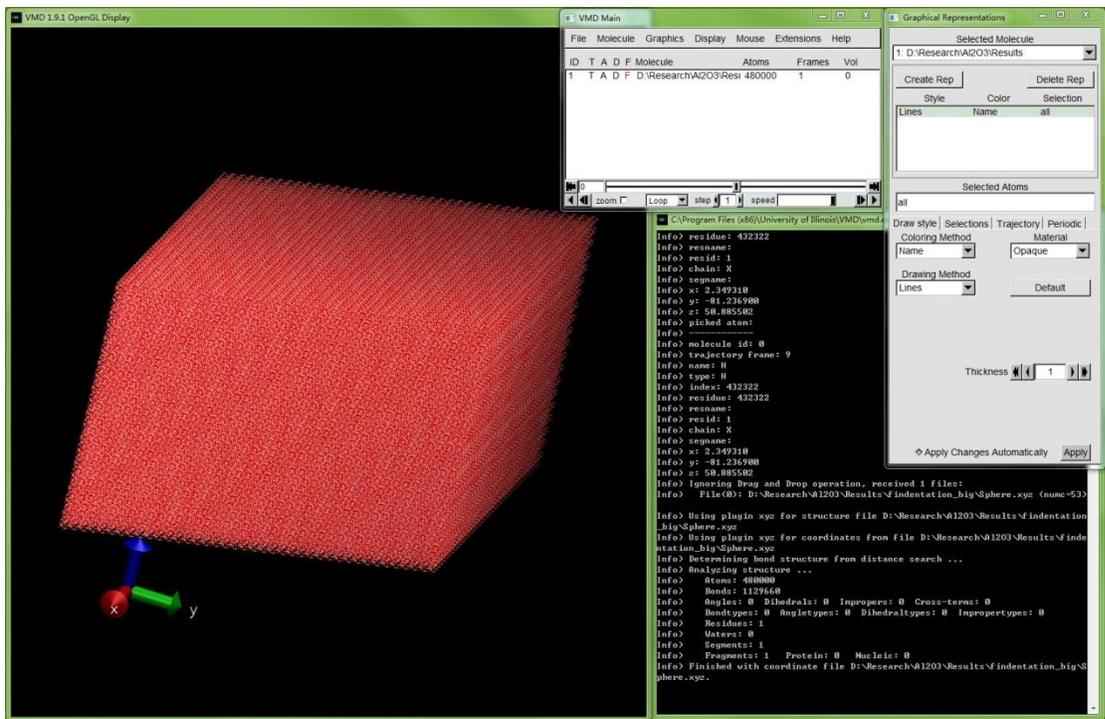


Figure 1-5. VMD windows

## CHAPTER 2 SIMULATION MODEL AND FORCE FIELD

### Force Field

In my study, a simple transferable interatomic potential model called modified-Matsui potential. This potential is first proposed by M Matsui, a Japanese researcher, in 1996. [9] In 2006, a Chinese scholar named Jizhong Sun made a work of simplification and modification of this potential. [10] This work make the parameters needed from 7 to 5 and some results including the lattice constants and position parameters be more accurate to the experiment. But for the elastic constants Sun admitted this potential is not good enough. Figure 2-1 shows the table in Sun's paper to compare its result to previous work and experiment measurement results.

In this work, the modified-Matsui potential is adopted as the potential for the simulation. This is a pair potential can be described in Eq. 2-1. The individual terms represent Coulomb, van der Waals and repulsion interaction. [10]

$$V(r_{ij}) = \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} - \frac{C_{OO}}{r_{ij}^6} + A_{OO} \exp\left(-\frac{r_{ij}}{\rho_{OO}}\right) + A_{MO} \exp\left(-\frac{r_{ij}}{\rho_{MO}}\right) \quad 2-1$$

The parameters for aluminum oxide are shown as in Table 2-1.

In LAMMPS, we can find the formula corresponding to this potential energy. LAMMPS call it the potential of Buckingham with Coulombic term. That means we can use LAMMPS command to assign the parameters' values. Eq. 2-2 is the Buckingham potential in LAMMPS. And Eq. 2-3 is the formula for Coulombic term.

$$E = A e^{-r/\rho} - \frac{C}{r^6} \quad r < r_{c1} \quad (2-2)$$

$$E = \frac{C q_i q_j}{\epsilon r} \quad r < r_{c2} \quad 2-3$$

We can notice that for each part of the potential, cutoff is needed. Meanwhile, neither M Matsui nor Sun said anything on the cut off issue, especially the cutoff for Coulombic term. Since we know Coulombic force dominates the interaction force when 2 ions is far away from each other.

In consideration of accuracy and make sure the simulation can be done without the neighbor list overflow error, there cutoff values are used in my research. We pick  $r_{c1}=12$  Angstrom, and  $r_{c2}=14$  Angstrom. They are the maximum value to make sure the simulation runs successfully.

While there are also two main limitations of this potential: One is it is only available to simulate the (0001) surface. The other is as the Figure 2-1 shows, it is not accurate in elastic constants.

The first limitation has been mentioned in Sun's conclusion. [10] But during my research I once did some attempts to do other simulation with other surface as the free surface. But the atoms in the model cannot in the right position. So that's why I only do the simulation with (0001) surface as the free surface and make other surface as periodic.

The other advantage is the excellent agreement on the lattice constants ( $a$  and  $c$ ) and the positional parameters ( $u$  and  $v$ ) with the experimental results. And the disadvantage is the elastic constants are not accurate enough, and that may leads to the inaccurate of the results of simulation. While, the elastic constants are in the same order of magnitude with the ones come from experiments. For simulation, that difference is acceptable, and the result can be used to do analysis qualitatively.

While neither J.Z Zhang nor Matsui provided the cutoff in their study. Taking the accuracy and limitation of neighbor list, we take the cutoff value as 14 angstrom, which is the largest value to make sure the simulation running without the neighbor list over flow issue.

## **Simulation Model**

### **Crystal Structure of $\alpha$ -Al<sub>2</sub>O<sub>3</sub>**

When doing the modeling of corundum, we should figure out the crystal structure of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>. In chapter 1, we mentioned the crystal structure and the lattice constants. In this case, we can consider the  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> has the HCP crystal structure with lattice constant  $a=4.7602$  Angstrom and  $c=12.9933$  Angstrom. [11] Figure 2-2 shows the general view of the crystal structure of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>. [12]

### **Primitive Cell of $\alpha$ -Al<sub>2</sub>O<sub>3</sub>**

The primitive cell of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> has 10 atoms, containing two formula units of aluminum oxide. The aim to introduce the primitive cell is too make sure the unit cell used to build the simulation model is correct. Figure 2-3 shows the primitive cell structure from different views.

### **Unit Cell**

Figure 2-4 shows what the unit cell used in this study looks like in different orientations. This is a 30-atom unit cell, and it is roughly 1/3 of HCP structure. That is shown in Figure 2-5. So we can use the lattice constants to be the parameters needed in building model. This unit cell is a good bridge connecting the material to the computational modeling.

## Building Model

The principle of building model is shown in Figure 2-6. The  $a$  and  $c$  values are come from Sun's paper, which is shown in Table 2-2. The unit is Angstrom. The unit cell which is marked by red and pink is repeated every  $a$  length in the 2 directions which has 120 degree angle with each other, and repeated every  $c$  length to the direction perpendicular to the that two directions.

The general procedure of model building is shown in Figure 2-7.

Figure 2-8A is made to make sure the model I made is correct by comparing with previous work. Figure 2-8B is used for comparing with my model. [13] Note that in Figure 2-8A, the bigger pink ball, which represents the atom of Al, is the same as the little ball in Figure 2-8B. And the red smaller ball, which represents the atom of oxide, is the same as the big ball in Figure 2-8B.

Table 2-1. Potential parameters for aluminum oxide

Ionic-Ionic	A(eV)	$\rho(\text{\AA})$	C(eV/ $\text{\AA}$ )
Al <sup>3+</sup> -O <sup>2-</sup>	3411.118	0.244549	0
O <sup>2-</sup> - O <sup>2-</sup>	91.55955	0.547148	32.32

Table 2-2. Lattice constants

Lattice constants	Experimental Measurement( $\text{\AA}$ )	Potential fitting( $\text{\AA}$ )
$a$	4.7602	4.7727
$c$	12.9933	12.99

Calculated and experimental values for  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>

	Exp [23]	Matsui [15]	Bush et al. [18]	This work
$a$ (Å)	4.7602	4.71	4.82 <sup>a</sup>	4.7727
$c$ (Å)	12.9933	13.14	13.01 <sup>a</sup>	12.9900
$u$	0.35212	—	0.35623 <sup>a</sup>	0.35566
$v$	0.30624	—	0.29743 <sup>a</sup>	0.30150
$C_{11}$ (10 GPa)	49.69	—	60.72	71.45
$C_{12}$ (10 GPa)	16.36	—	32.22	32.75
$C_{33}$ (10 GPa)	49.80	—	60.65	70.93
$C_{44}$ (10 GPa)	14.74	—	9.53	9.97
$C_{13}$ (10 GPa)	11.22	—	—	18.78
$C_{66}$ (10 GPa)	19.35	—	—	19.35
$K_0$ (10 GPa)	25.2	25.8	—	39.11
$E_{\text{latt}}$ (eV)	-321.4 <sup>b</sup>	-89.0 <sup>c</sup>	-315.19	-321.36

Figure 2-1 Result comparison of different potentials and experimental measurement

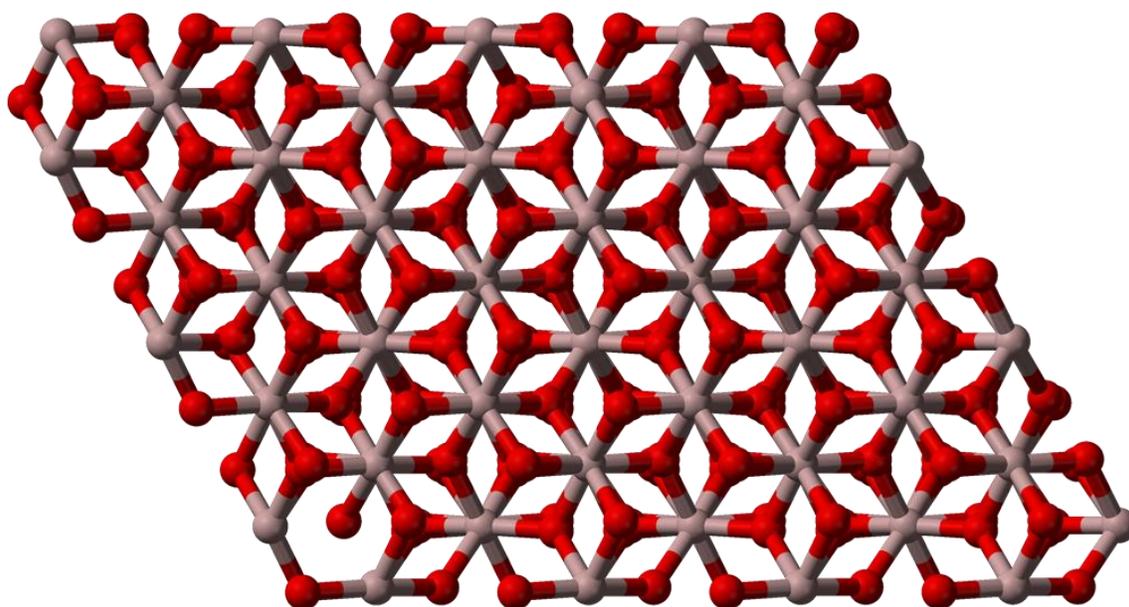


Figure 2-2 General view of the crystal structure of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>. (Source: <http://en.wikipedia.org/wiki/File:Corundum-3D-balls.png>).

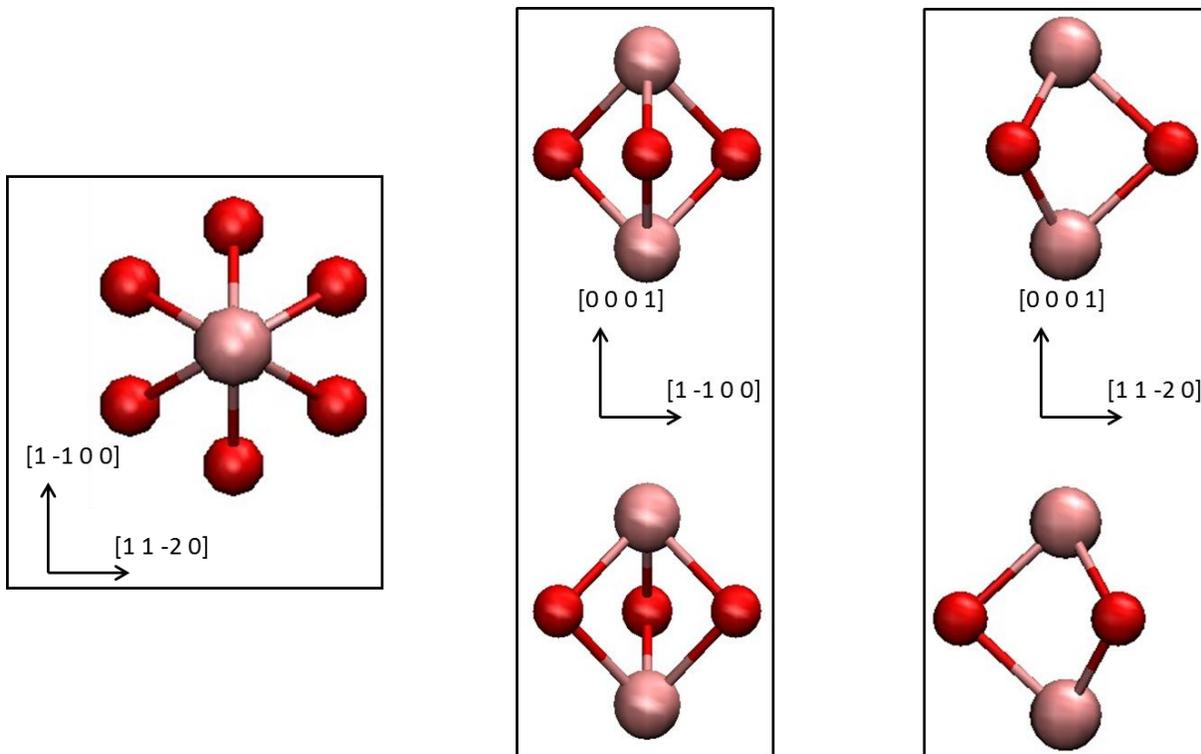


Figure 2-3. Primitive unit cell of  $\alpha\text{-Al}_2\text{O}_3$

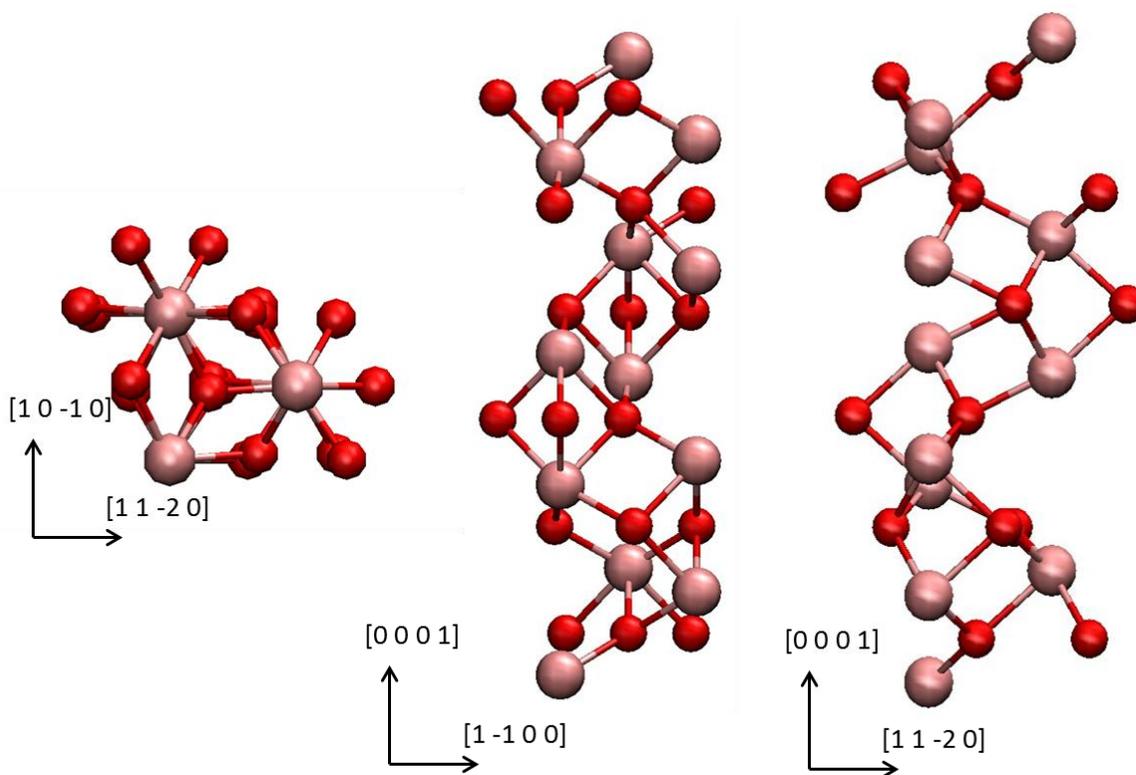


Figure 2-4. Unit cell used in the simulation modeling

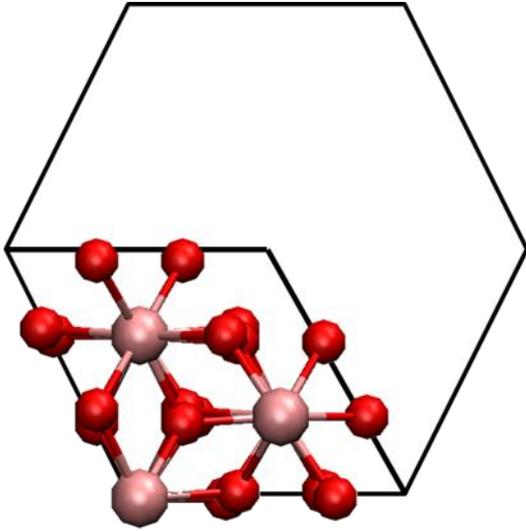


Figure 2-5. Top view for unit cell in HCP structure

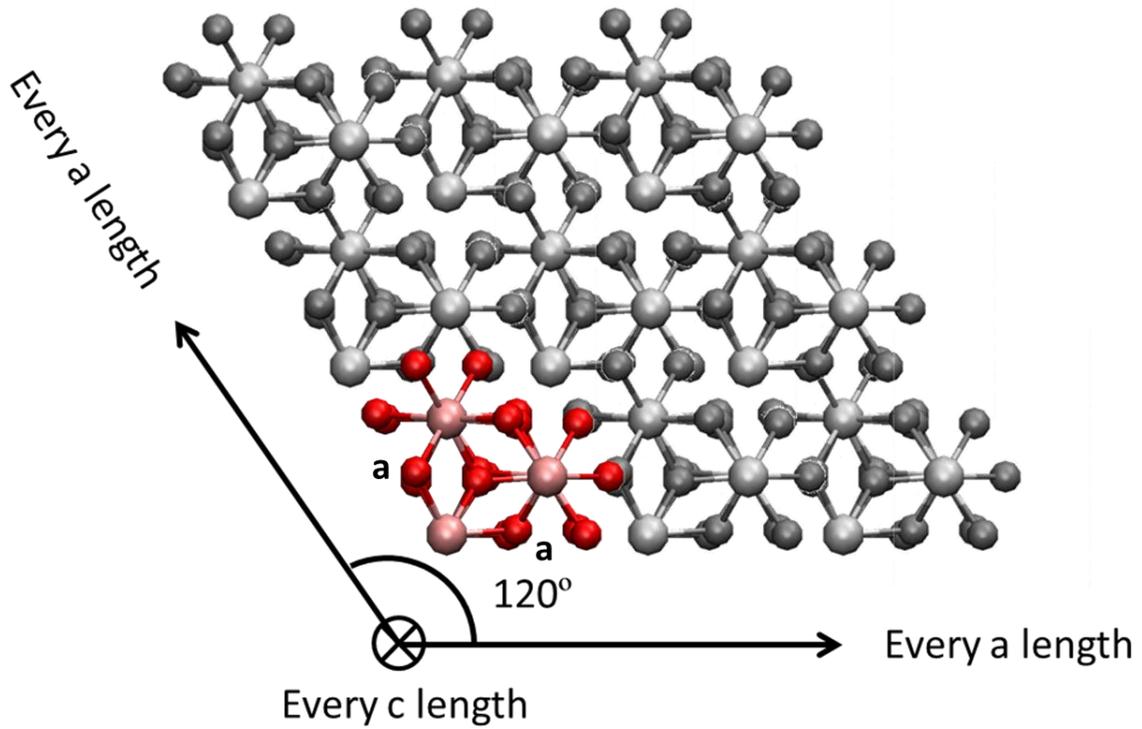


Figure 2-6. The general method of building the model

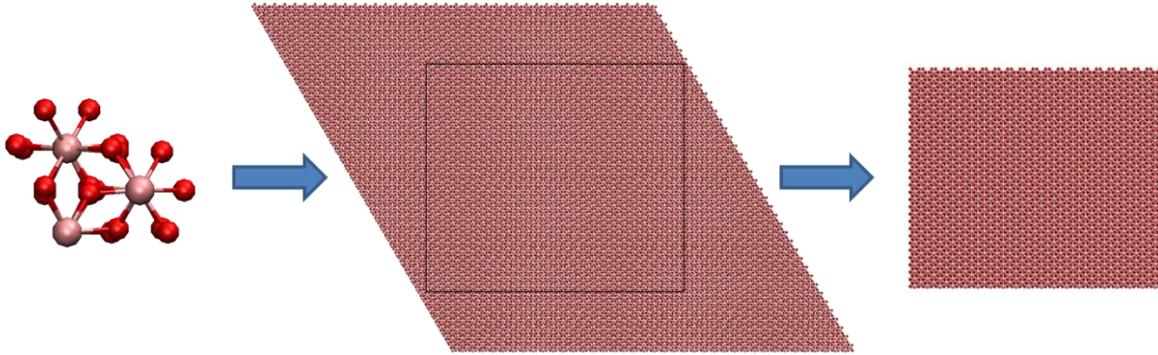


Figure 2-7. Procedure of model building

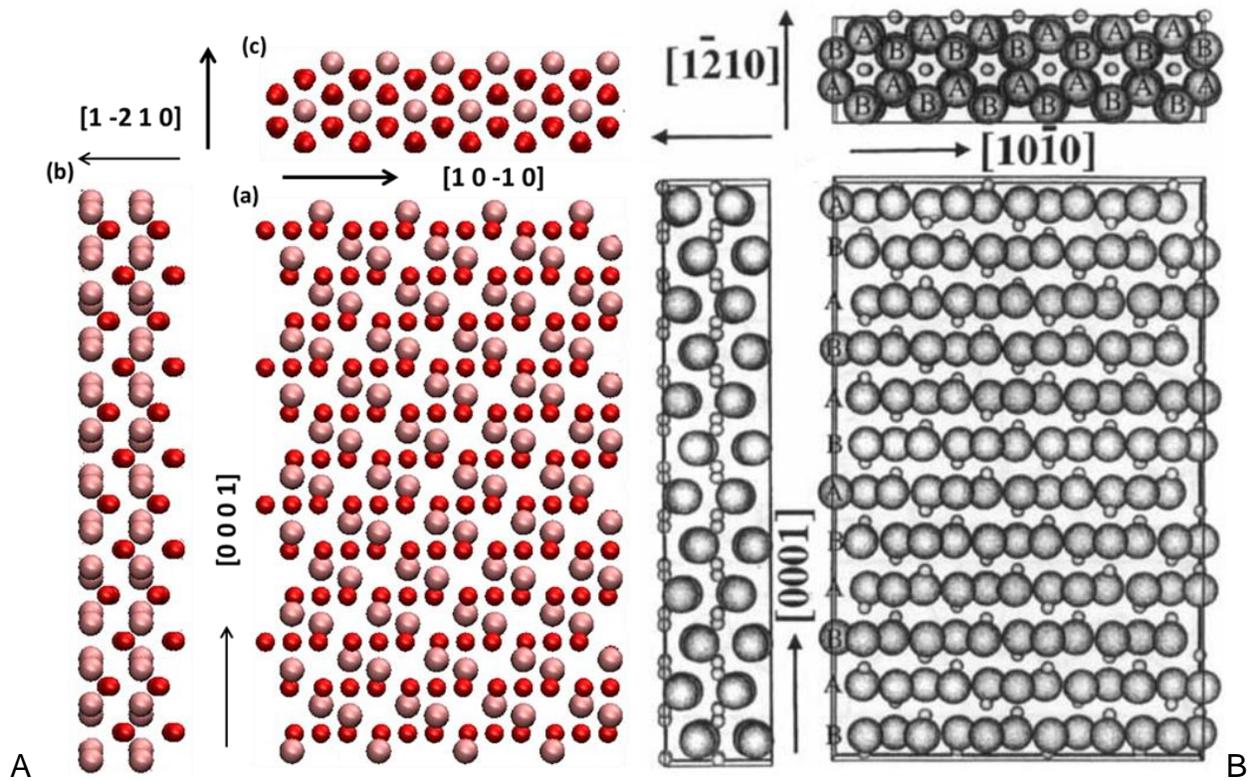


Figure 2-8. Comparison with my work and the view of previous work. A) The view of my model B) The view of previous work model

## CHAPTER 3 SIMULATION RUNS AND RESULTS

### **Simulation Procedure**

Since in LAMMPS and VMD, there is no HCP coordinates, so I change it to Cartesian coordinates. The correspondence relationship between HCP coordinates and Cartesian coordinates are shown in Table 3-1. At the right of the Table 3-1, the dimension information specimen I used in this study is shown.

In my simulation, I set the x y boundaries as periodic boundaries conditions and leave the z surface as the free surface. The Nose-Hoover thermostat is used to maintain the constant temperature about 0K. The velocity-Verlet algorithm with a time step of 1 fs is used for time integration.

Figure 3-1 is the sketch of how the loading added on the specimen. The blue boxes are used to show the effect of periodic boundary conditions. The loading velocity is 0.02 Angstrom/picosecond. And the radius of the indenter is 500 angstrom.

In the simulation I set the x y surfaces as periodic boundaries. And leave the z surface as the free surface. The Nose-Hoover thermostat is used to maintain the constant temperature at 0K. The velocity-Verlet algorithm with a time step of 0.001 ps is used for time integration.

### **Loading Progress**

Figure 3-2 is the loading-displacement curve. At point A there is an obvious change and we can find the curve changes here. The value of force grows with the indentation depth increases, and drop down at a point. To analysis the atomic structure change, we pick up two critical points. They are A and B, shown on the curves. B is a

random point far away from point A. And then, I will show you the atomic structure change during the loading progress.

Figure 3-3(A-F) are to show the atom structure changes along the indentation depth increasing. Figure 3-3D shows that the status of atoms changed dramatically at point A. Figure 3-3F is the status of atoms at the end of loading progress. Since during the loading progress, dislocation is observed, so we need to unload it and do RDF analysis to figure out other atomic structure changing like phase transition or amorphization. Before the RDF analysis, fully unloading is needed.

### **Loading-Unloading Progress**

Figure 3-4 is the Loading-Unloading progress load-displacement curve. Unloading is made at point B. Figure 3-5(A-F) show the atom structure changes along the indentation depth increasing. Figure 3-5(A-E) are exactly same as Figure 3-3(A-E), showing the loading progress. At the time of Figure 3-5F, the displacement is negative, which means the indenter has been above the initial position, and the atoms are still very messy. From this view, I didn't find any dislocations. That means there is phase transition or amorphization happening. The RDF analysis is done.

For the Figure 3-6(A-C), the red curves stand for the RDF curves before loading, which means the  $\text{Al}_2\text{O}_3$  is alpha phase. And the blue ones are the curves from RDF analysis for the deformed and no loading specimen.

Figure 3-7(A-C) are the comparisons with the RDF curves of deformed specimen with the amorphous Alumina. Since what we saw in Figure 3-3 and Figure 3-5, the specimen is partially amorphous, not wholly. But LAMMPS made an average calculation, that leads the curves have some information of alpha phase alumina. After comparison with the figures, it is easy to find that the blue curves do have a trend from the red ones

to the black ones. And at some area the RDF values are reduced significantly. So from this analysis we can claim that the pressure induced amorphization happens during the loading progress.

### **Loading-Holding Progress**

In the loading-unloading progress I find that after fully unloading, the displacement is negative. The explanation for this observation is that the amorphization leads the alumina density change, and then make the specimen volume expand. To further check this explanation, I do another case called loading-holding progress, which means loading before point A and keep the indentation depth at a constant, and see the load-time curve. The load-time curve is shown in Figure 3-8.

Figure 3-9 (A-E) is to illustrate the atomic structure change with the simulation time increasing. In Figure 3-9d, we can find, although we stop the indentation loading, the progress of amorphization does not stop. At the end of the progress, the force is much bigger than the one at point A, where we stop the indentation.

Since the density of amorphous alumina varies over an exceptionally range, between  $2.1 \text{ g/cm}^3$  and  $3.5 \text{ g/cm}^3$ , [14] less than the alpha phase alumina  $4.0\text{-}4.1 \text{ g/cm}^3$ , which is studied in this study. So we can claim that the reason why there still have force between indenter and specimen the displacement is negative is the amorphization makes the specimen expand in volume, and all other faces are fixed. And then the specimen can only expand to the upward.

Table 3-1. Coordinates correspondence relations [10] and specimen dimension information

HCP coordinates	Cartesian coordinates	Length/lattice constants	Length/Angstrom
[1 1 -2 0]	x	20a	95.454
[1 -1 0 0]	y	$20^*(\sqrt{3}/2)a$	82.664
[0 0 0 1]	z	4c	51.96

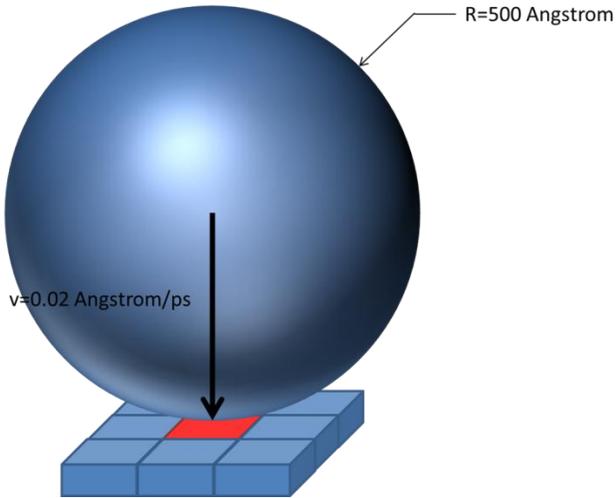


Figure 3-1. Sketch of how the loading added on the specimen

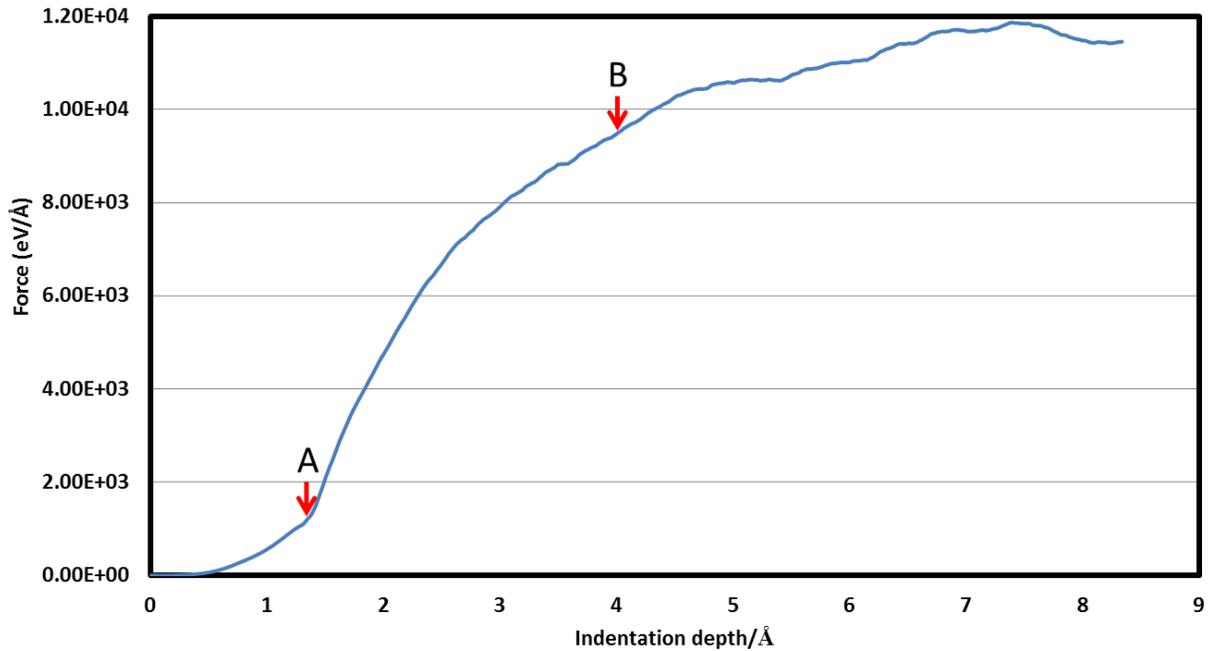


Figure 3-2. The loading-displacement curve of the loading progress

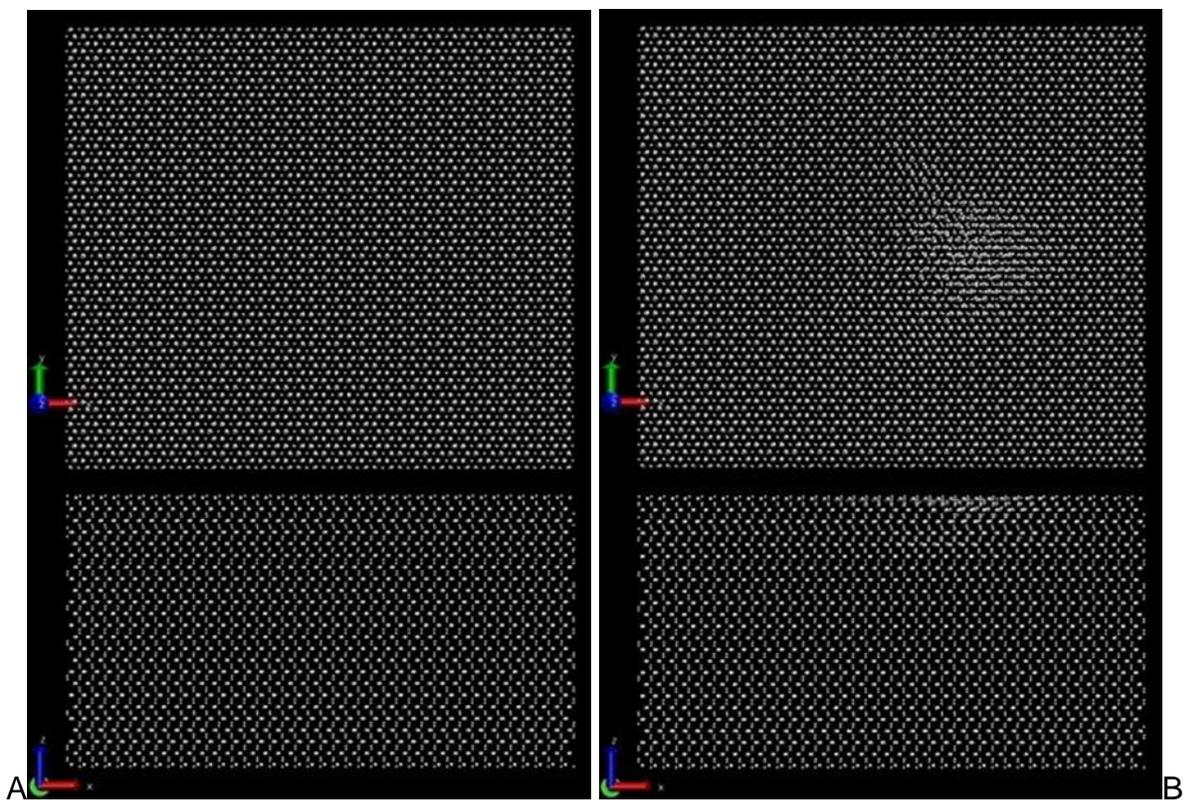


Figure 3-3. Atomic structures along the indentation depth increase. A) Depth=0Å, t=0ps.  
 B) Depth=1.22 Å, t=61ps. C) Depth=1.28 Å, t=64ps. D) Depth=1.48 Å, t=74ps  
 E) Dept=4.02Å, t=201ps. F) Depth=8.12 Å, t=406ps.

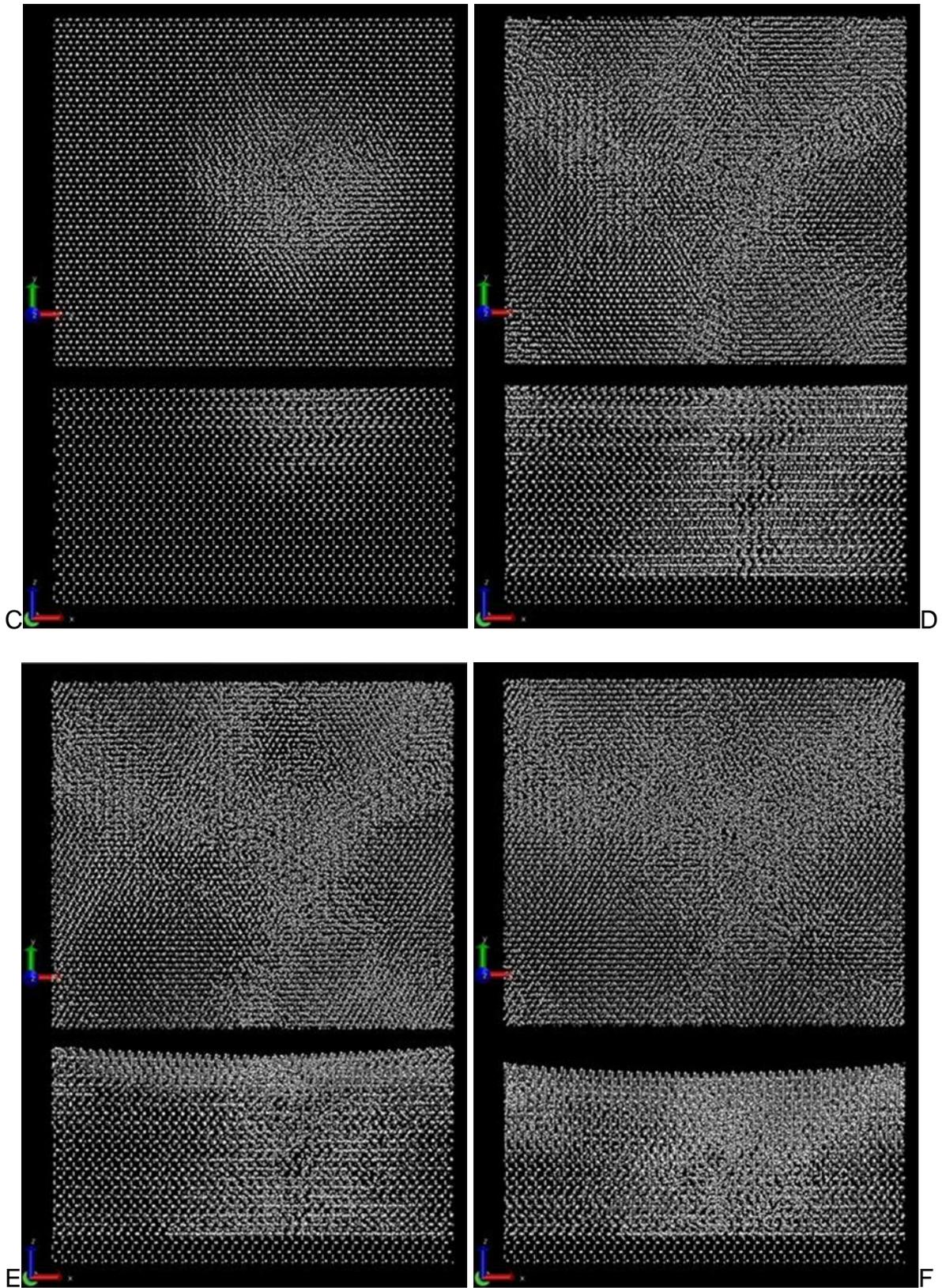


Figure 3-3. Continued

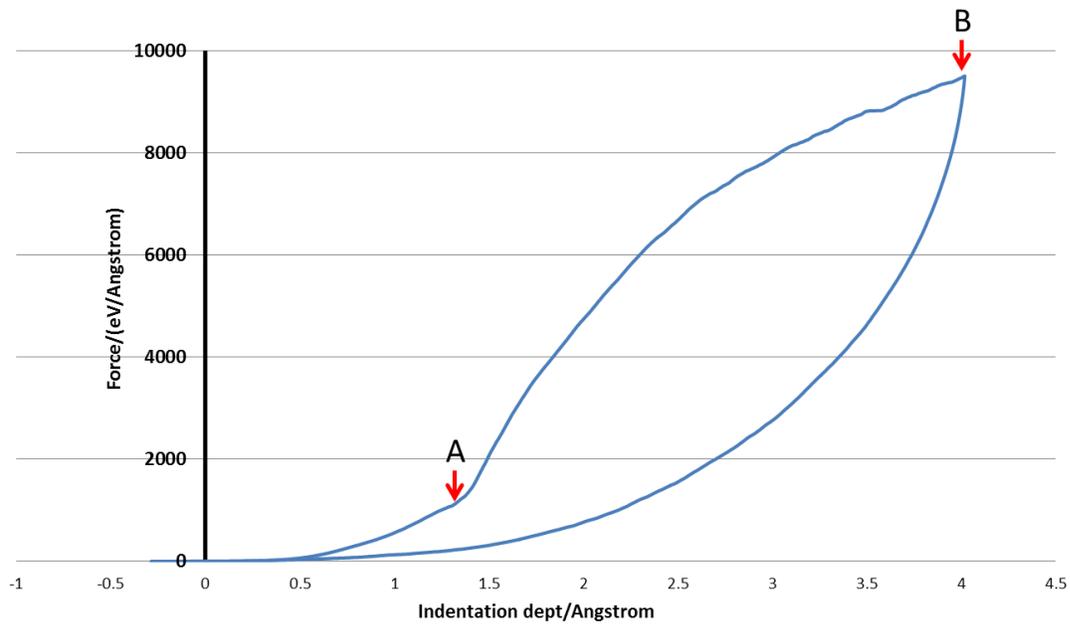


Figure 3-4. The Loading-Unloading progress load-displacement curve

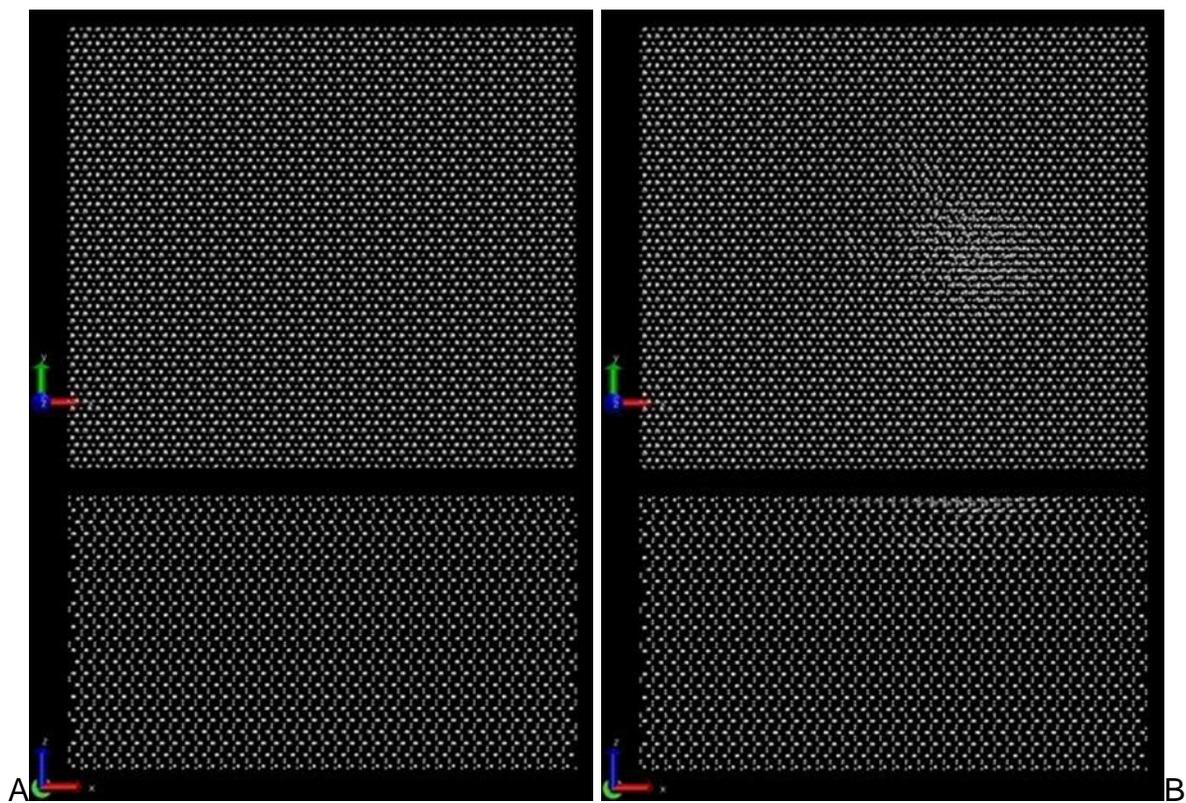


Figure 3-5. Atomic structures along the indentation depth and time change. A) Depth=0Å, t=0ps. B) Depth=1.22 Å, t=61ps. C) Depth=1.28 Å, t=64ps. D) Depth=1.48 Å, t=74ps E) Depth=4.02Å, t=201ps. F) Depth=-0.29 Å, t=404ps.

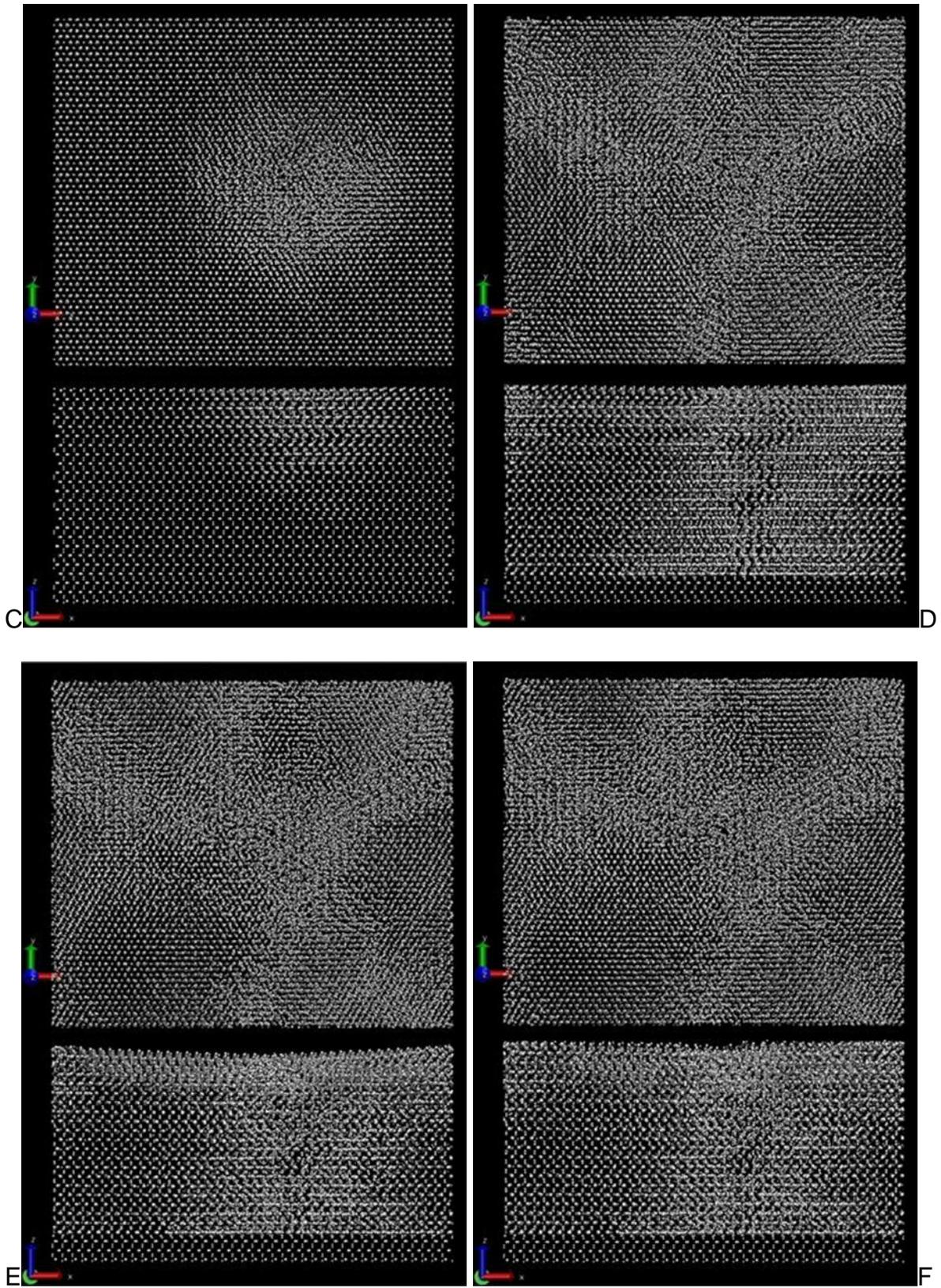


Figure 3-5. Continued

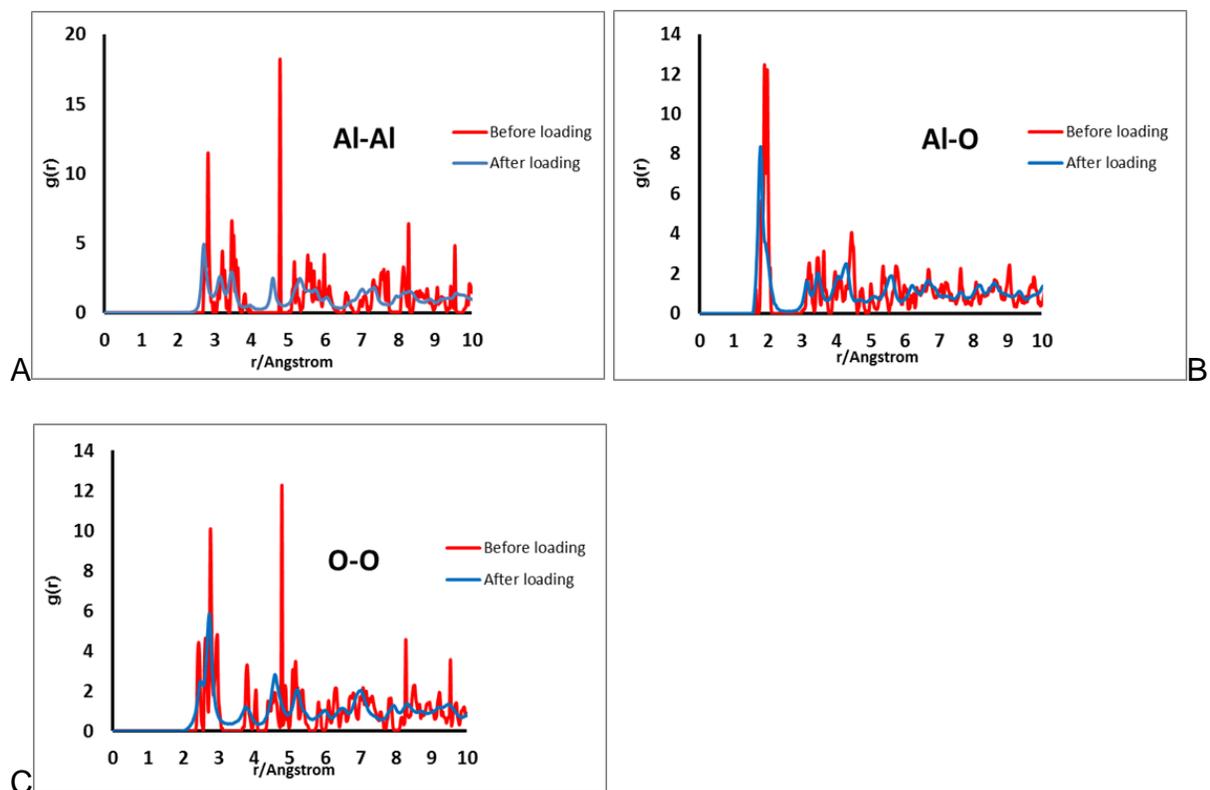


Figure 3-6. The comparisons with the RDF curves of perfect alpha phase alumina with the deformed specimen. A) Al-Al. B) Al-O. C)O-O.

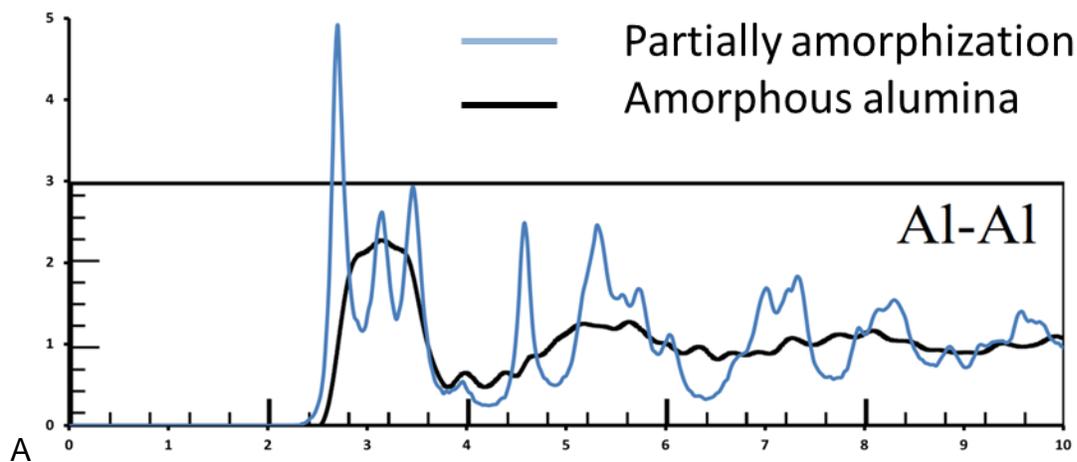


Figure 3-7. The comparisons with the RDF curves of deformed specimen with the amorphous alumina. A) Al-Al. B) Al-O. C)O-O.

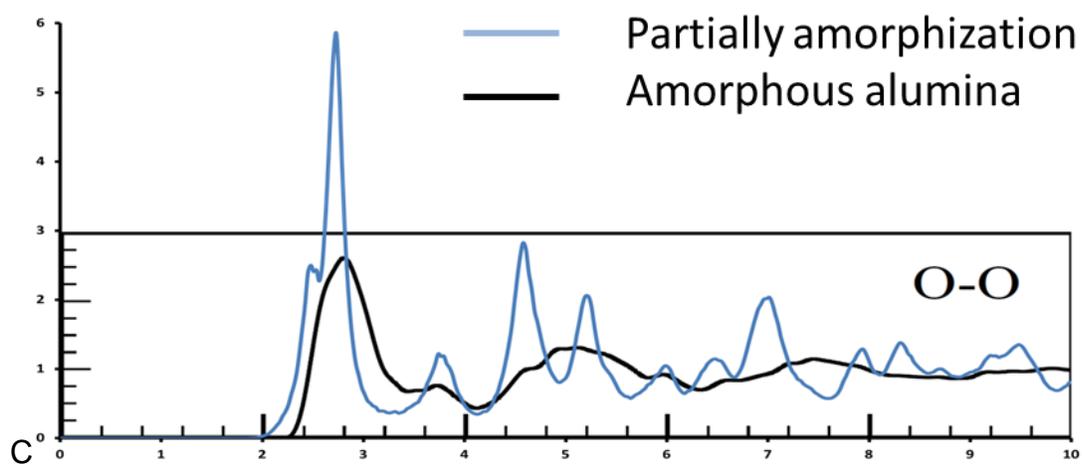
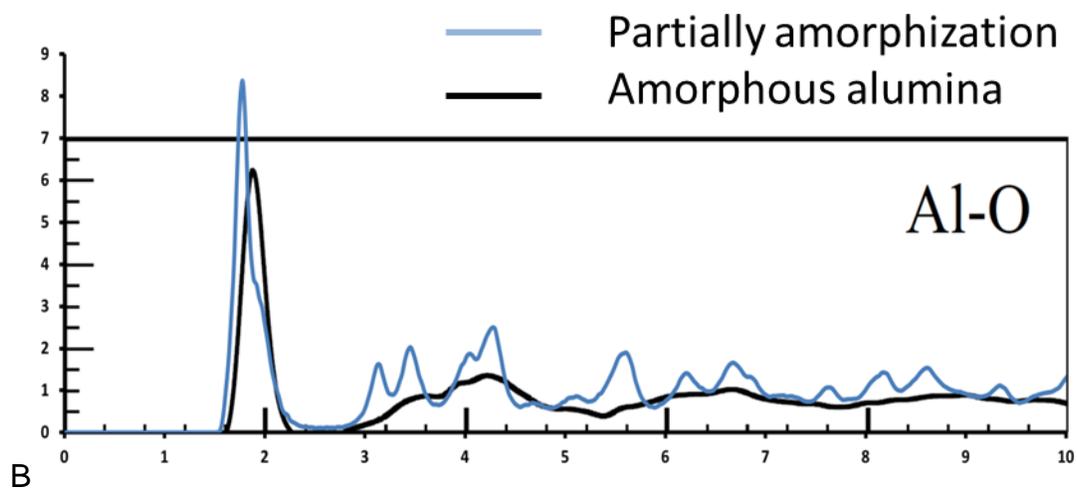


Figure 3-7. Continued

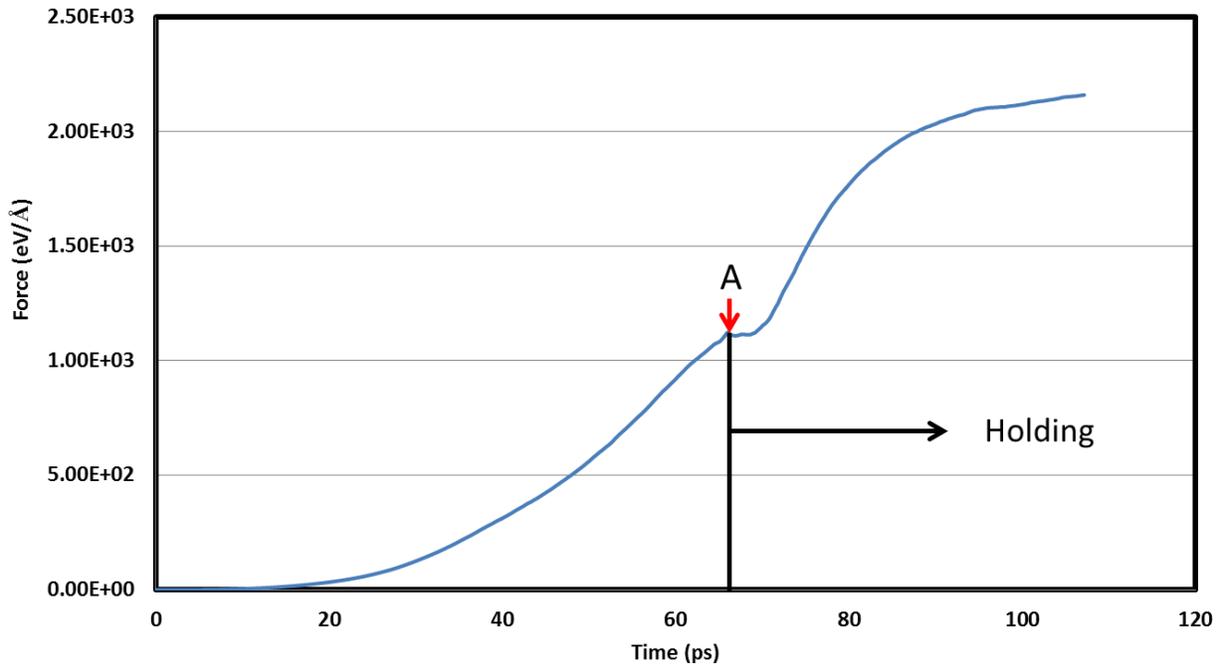


Figure 3-8. Loading-Holding progress load-time curve

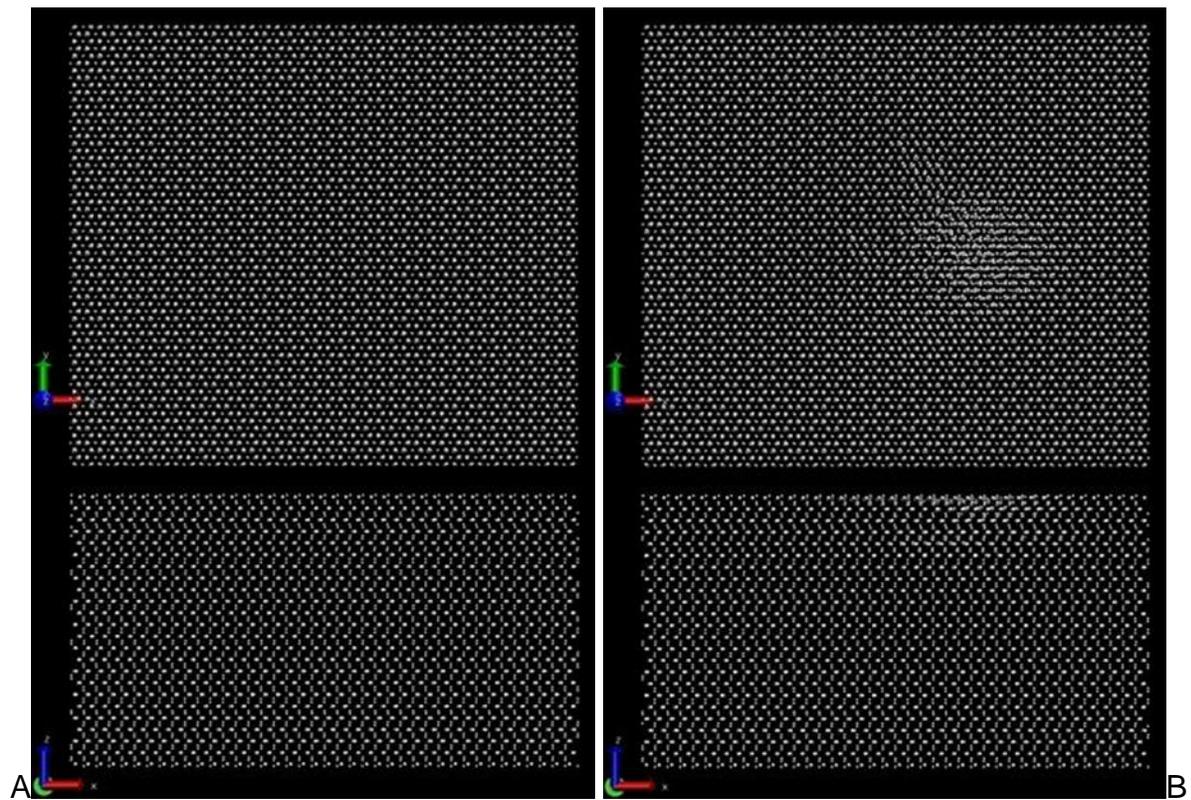


Figure 3-9. Atomic structure change with the simulation time increasing. A)  $t=0\text{ps}$ . B)  $t=61\text{ps}$ . C)  $t=64\text{ps}$ . D)  $t=74\text{ps}$ . E)  $t=112\text{ps}$

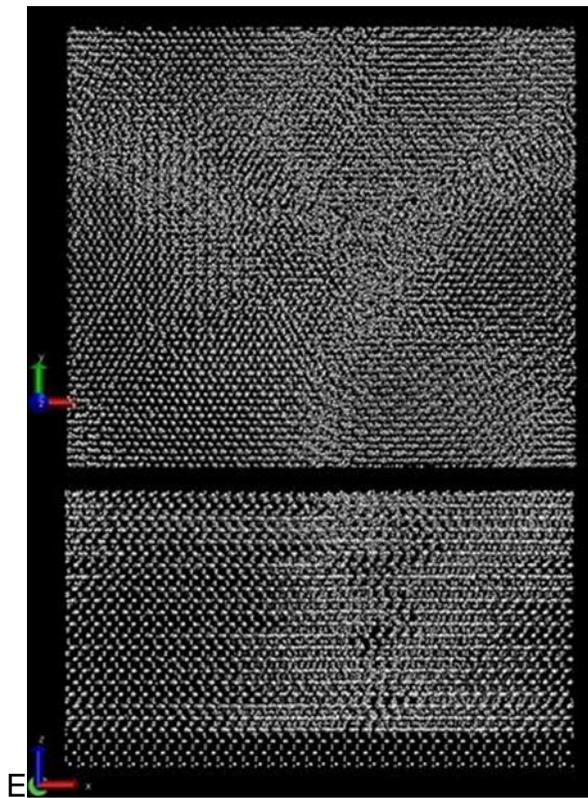
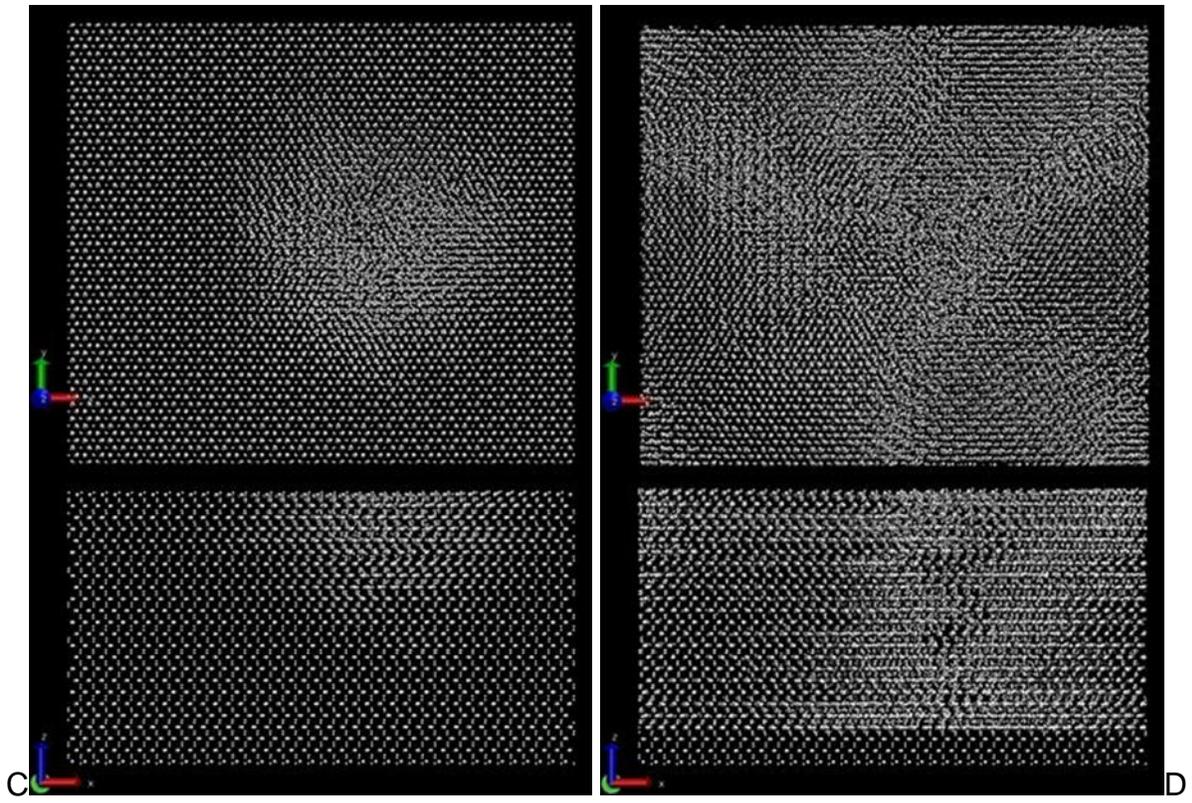


Figure 3-9. Continued

## CHAPTER 4 CONCLUSIONS AND DISCUSSIONS

### Conclusions

After 3 cases of simulation, we can have 2 conclusions below:

- Under the loading rate of  $\sim 10^8$  nanoindentation in MD simulation, no obvious dislocation or phase transition has been observed within the model of nanoscale-thickness corundum thin film.
- Instead, the amorphization happens with a volumetric expansion.

### Discussions

To discuss why the observations do not have the agreement with the experiment, some discussions were made. There are 3 possible reasons

**Potential problem:** For MD simulation, to some extent, the potentials decide the result. It is possible we can only get this result using this potential for the nanoindentation test.

**Strain rate effect:** The strain rate is too big. Nearly  $4.5 \times 10^8$  high velocity test. Material behaviors will differ from the test in load velocity. Material behaviors will differ from the test in load velocity.

**Size effect:** The size of the specimen and the indenter are much smaller than the ones in experiments.

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## BIOGRAPHICAL SKETCH

Chen Zhang was born and raised in Jinzhou, China. He graduated from Harbin Engineering University in 2011 with a Bachelor of Science in engineering mechanics. Chen came to Gainesville, Florida in 2011 and was admitted to be a graduate student at University of Florida's Mechanical and Aerospace Engineering Department. He received his M.S. degree from the University of Florida in the spring of 2013. Chen enjoys swimming and eating.