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Research Paper

# **The Computational Study of Number of Shot Particles and Distance Effects on Residual Stress and Mechanical Behavior of Ti-6Al-4V Alloy after Shot Peening Process: Molecular Dynamics Approach**

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## **Abstract**

Various parameters can affect shot peening such as the number of particles and distance between particles and the surface layer. In this computational study, these parameters' effects on the creation of residual stress and mechanical behavior of Ti-6Al-4V alloy were described. For this purpose, Molecular Dynamics (MD) method is applied in two main steps. First, the simulated titanium surface was equilibrated for 1 ns. Next, the shot peening process was done on the equilibrated surface by using the various numbers of particles and distance. MD simulation results indicated, that by increasing the number of particles from 1 to 5, the mechanical behavior of the titanium surface was improved, and residual stress and hardness of the surface increased and reached 452.02 MPa and 494.46 HV in model 1 (Lj potential between particle and titanium surface), respectively. Furthermore, the results indicated that decreasing the distance from 15 Å to 5 Å led to increasing compressive residual stress and hardness of titanium surface mechanical. Numerically, by decreasing the shot peening distance from 15 Å to 5 Å, residual stress and hardness of titanium surface layer increased and reached -419.63 MPa and 510.83 HV in model 1, respectively.

## **Keywords**

Shot Peening, Residual Stress, Interatomic Force-field, Mechanical Improvement, Embedded Atom Model, Lennard-Jones Potential

## **1. Introduction**

The shot peening process is an effective procedure implemented to modify the mechanical properties of metals and composites. It entails striking a surface with round particles with force sufficient to create plastic deformation [1-2]. Technically, this process is used to strengthen and relieve stress in various structures such as steel automobile crankshafts and connecting rods. Shot peening is similar mechanically to sandblasting, though its purpose is not to remove material [3-4]. Rather, it employs the mechanism of plasticity to achieve its target, with each particle functioning as a ball peen hammer. Historically, this process was used in forging processes as early as the Bronze Age to strengthen armor, swords, and tools. Gun barrels in the civil war were subject to peening to increase the hardness

of Damascus steels, and the fillets of crankshafts in early European race cars were hand-peened with specially-made hammers by 1922 [5-6]. Today, this promising method is implemented in various industrial aims for mechanical behavior improvement of metal and alloy-based structures [7-8]. In previous research, Unal et al [9] reported the fatigue behavior of Ti-6Al-4V alloy is tend to be improved by severe plastic deformation via shot peening and plasma nitriding. Shot peening with sub-branches: Conventional shot peening (A12-14), severe shot peening (A28-30 and A34-36), and re-peening (N6-8) are exposed in this experimental work. Besides plasma nitriding is implemented at 500 °C, 550 °C, and 600 °C with durations of 4, 8, and 16 h. Results indicated that severe plastic deformation by severe shot peening generally triggers the formation of a thicker compound layer and emerges distinct diffusion depth with finer and oriented precipitation. Also, the phase's intensity obtained from XRD peaks has been amplified by the application of prior shot peening. Kumar et al. [10] studied the effect of ultrasonic shot peening (USSP) on microstructural modification in the surface region and low cycle fatigue (LCF) behavior of the Ti-6Al-4V alloy, at room temperature. They conclude the nanostructure of 17-25 nm was developed in the surface region of the alloy by USSP. Furthermore, the fatigue life of the USSPed samples was found to increase progressively with the decrease in strain amplitude to a much larger extent in comparison with those of the non-USSPed ones. In another experimental study, Liu et al. [11] investigated the structure features and grain refinement of alpha phase in coarse-grained Ti-6Al-4V subjected to surface severe plastic deformation by using high energy shot peening (HESP). The results of this study indicated promising deformation-induced structure response characteristics, including the markedly reduced contribution of twinning to deformation of coarse-grained alpha phase with hexagonal close-packed (HCP) structure. Yang et al. [12] studied an experimental investigation on the fretting wear of Ti-6Al-4V by using a self-designed test machine. The wear morphologies and the cracking phenomena of as-received and shot-peened specimens were comparatively analyzed by combining the applications of a laser scanning confocal microscope and a scanning electron microscope. Their results showed that shot peening exhibited an increase in the wear volume during the early fretting wear period, while it reduced the material loss in the long-term fretting wear process.

In addition to experimental methods, computer simulations have a high ability to study the shot peening process [13-14]. Molecular Dynamics (MD) simulation is one of the appropriate methods to describe the mechanical improvement of alloys after the shot peening procedure [15-17]. MD is a computer simulation approach for describing the displacement of particles (molecules or atoms). In this computational method, various particles are allowed to interact for a fixed period, giving a view of the dynamic evolution of the simulated system. In previous computational research, this method was used successfully for the shot peening process description. For example, in the study by Moradi et al. computational method was used to investigate the effect of velocity and diameter of particles effects on the mechanical behavior of Ti-6Al-4V surfaces improved in the shot peening process, [18]. In this study, two types of force fields including the Embedded Atom Model (EAM) and Lennard-Jones (LJ) were implemented to model the colliding atoms, which yielded almost similar results. The effect of increasing hardness of the surface was observed with increasing particle velocities and diameters. Furthermore, Wang et al. [19] used the MD approach to examine the effect of particle size and collision angle in the surface mechanical attrition treatment (SMAT). In this study, silicon matrix and diamond spheres were used for MD simulation. Wang et al. introduced the parameters which play

a fundamental and direct role in the mechanical process. This process is similar to the shot pinning procedure and has been well described by using atomic simulations. Based on these research outputs, as the magnitude of the collision particles in the matrix increases, the amount of stress applied to the atomic matrix enlarged, too. Through these researches study, we conclude the particle number and distance effects on the shot peening process were not reported. So, in the current MD study, we describe these parameters' effects on the mechanical behavior of Ti-6Al-4V alloy after the shot peening procedure. For this purpose, MD simulations were done with Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) in 2 main steps [20-21]. Firstly, the simulated structures such as pristine alloy matrix and shot peening particles (carbon steel particles) equilibrated for 1 ns. After equilibrium phase detection in simulated structures, the shot peening procedure was implemented to Ti-6Al-4V alloy, and the mechanical properties of simulated atomic samples were reported. In this study, the effect of several shot particles and the distance of shot particles from the surface on residual stress, and the Mechanical Behavior of Ti-6Al-4V Alloy in the shot peening process have been investigated with molecular dynamics simulations which have not been investigated in the previous researches.

## 2. Computational Details

MD simulation is a prevailing tool to explore the dynamics of nanostructures based on Newton's laws for various atomic compounds [22-23], for example, the mechanical behavior of alloys. Conventionally, these simulations define the particle trajectories by solving Newton's law, because of forces between particles. In this work, we used the exact atomic model to study the Ti-6Al-4V alloy mechanical properties after the shot peening process. Considering the importance of interatomic potential in MD simulation results, the EAM force field has been applied in the atomic description of Ti-6Al-4V alloy and shot peening particle structures [24-25]. In the EAM force field, possible energy for atoms arrangement is represented by a superposition of the interactions' distance component. Theoretically, the common description of the EAM force-field is [24-25],

$$E_i = F_\alpha \left( \sum_{j \neq i} \rho_{\alpha\beta}(r_{ij}) \right) + \frac{1}{2} \left( \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij}) \right) \quad (1)$$

In this equation,  $r_{ij}$  is the distance between atoms  $i$  and  $j$ ,  $\phi_{\alpha\beta}$  is a pair-wise potential function,  $\rho_{\alpha\beta}$  is the contribution to the electron charge density from atom  $j$  of type  $\beta$  at the location of atom  $i$  of type  $\alpha$ , and  $F_\alpha$  is an embedding function that represents the energy required to place atom  $i$  of type  $\alpha$  into the electron cloud. Atomic interaction between shot peening particle and pristine matrix described by using 2 groups of force-fields. In MODEL 1, this interaction is described by using LJ model. But in MODEL 2, this atomic interaction is described by using EAM model. LJ force-field is described below [26],

$$\phi(r_{ij}) = 4\varepsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right] \quad r_{ij} \leq r_c \quad (2)$$

Where,  $\varepsilon$  constant represents the depth of the potential well,  $\sigma$  constant shows the finite atomic distance at which the potential function is zero, and the distance between the atoms is represented by

$r_{ij}$ . In this equation, the cut-off radius is shown with  $r_c$ , which is chosen as 12 Å in all of our calculations [27]. Table 1 shows the used interatomic force fields in the current computational study. In this study, two potential force fields including the embedded atom method (EAM) and Lennard-Jones (LJ) have been used for the simulation of atomic structures. The interaction between metal atoms in the simulated surface layer structure is described using EAM potential. The following equation expresses the EAM potential. The weak interaction between carbon steel shot particles and titanium surface is described LJ potential.

Table 1. Various force fields were implemented in the current MD study for shot peening process simulation

Model No.	Force-fields Between Various Structures		
	Titanium Matrix	Carbon Steel Particle	Titanium-Carbon Steel Particle
1	EAM	EAM	LJ
2	EAM	EAM	EAM

After determining the force-field for atomic structures inside the simulation box, the MD procedure was fulfilled. To describe the atomic displacement, Newton's second law at the nano-metric level is applied as the gradient of the interatomic force-field [28],

$$F_i = \sum_{i \neq j} F_{ij} = m_i \frac{d^2 r_i}{dt^2} = m_i \frac{dv_i}{dt} \quad (3)$$

$$F_{ij} = -grad V_{ij} \quad (4)$$

From equations (3) and (4),  $v$  is the velocity, the momentum  $P_i$  can be defined as the following [28],

$$P_i = m_i v_i \quad (5)$$

So, Energy (E) of the atomic structures can be expressed in the form of Hamilton as equation (6) [28],

$$H(r, P) = \frac{1}{2m} \sum_i P_i^2 + V(r_1 + r_2 + \dots + r_n) = E \quad (6)$$

Finally, the velocity-Verlet algorithm was applied to estimate the motion of the particles considering integrations form of Newton's law in equations (7), and (8) [29-30],

$$r(t + \Delta t) = r(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2 + O(\Delta t^4) \quad (7)$$

$$v(t + \Delta t) = v(t) + \frac{a(t) + a(t + \Delta t)}{2}\Delta t + O(\Delta t^2) \quad (8)$$

In both relations,  $r(t+\Delta t)$  and  $v(t+\Delta t)$  are the coordinates and velocities of particles at any time (respectively) and  $r(t)$ ,  $v(t)$  are the initial value of these physical parameters. Theoretically, various ensembles are used to create initial conditions in MD simulations. In our study, the canonical ensemble was obtained by applying the Noose-Hoover thermostat [31-32]. After the equilibrium process, the simulation continued for 1ns later, and the shot peening process was done in the MD box. After this process, the mechanical properties of the atomic matrix are described. So, simulations in our computational work consist of two main steps:

*Step 1: Equilibrium process of simulated structures:*

Initially, the Ti-6Al-4V alloys were simulated in the MD box with 200 Å, 200 Å, and 200 Å lengths in x, y, and z directions respectively. The Nose-Hoover thermostat was implemented to atomic structures to equilibrate them at  $T_0=300$  K as the initial temperature. In this step, the temperature, potential energy, and Radial Distribution Function (RDF) of simulated structures are reported in the equilibrium phase description. Figure 1 shows the simulated atomic structure in the initial step of the MD study. Also, the physical properties of pristine atomic structures are reported in Table 2. The mechanical properties of titanium matrix and carbon steel particles are mentioned in Table 3 and Table 4.

*Step 2: Shot peening process implementation to simulated structures:*

Next, after equilibrium phase detection in simulated structures, particles with various velocities and distances accelerated to the atomic matrix and so, the shot peening process was done in the MD box. After this atomic procedure was done, various output parameters such as maximum temperature, residual stress, the center of mass, departed atoms number, Vickers hardness, and roughness values are reported to investigate the shot peening process.

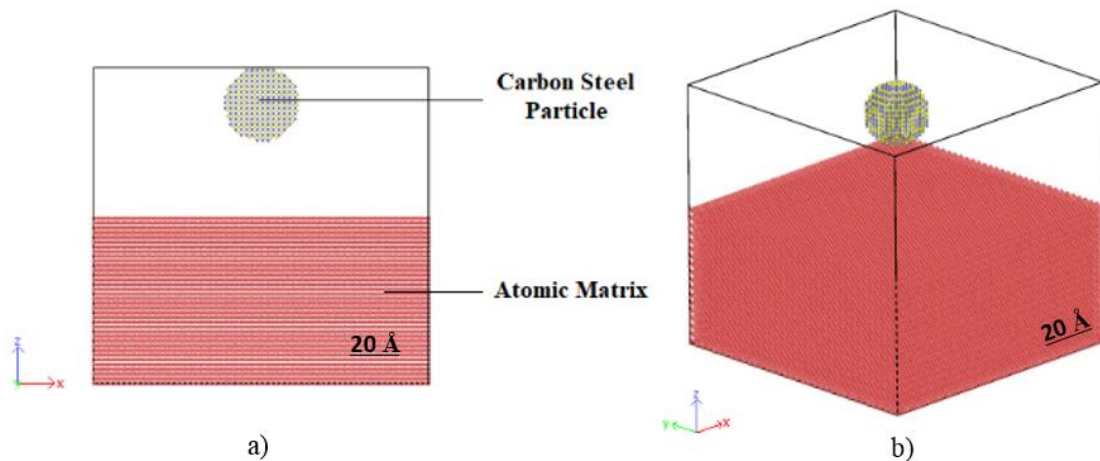


Figure 1. View of the titanium-based matrix and carbon steel particle in the shot peening process simulation at a) side and b) perspective views

Table 2. The MD simulation details and initial settings for the shot peening process

<b>Simulation Parameters</b>	<b>Value</b>
Simulation size	200×200×200 Å <sup>3</sup>
Initial temperature	300 K
Time step	0.001 fs
Number of atoms	137616

Table 3. The mechanical properties of Ti-6Al-4V

<b>Mechanical Properties</b>	<b>Value</b>
Density	4.43 g/cm <sup>3</sup>
Shear modulus	40 GPa
Tensile strength	180 MPa
Ultimate Strength	896 MPa
Yield Strength	827 MPa

Table 4. The mechanical properties of carbon steel shot particle

<b>Mechanical Properties</b>	<b>Value</b>
Carbon content (wt.%)	0.1%
Tensile strength	325 MPa
Yield Strength	180 MPa

### 3. Results and Discussion

#### 3.1 Equilibrium Phase of Simulated Structures

In the first step of the shot peening process study, the equilibrium of pristine matrix and carbon steel particles was reported. Technically, before the equilibration phase implementation, geometry optimization of these structures was done with Conjugate Gradient (CG) method [33-34]. This method is often used as an iterative process, applicable to sparse systems that are large to be done by a direct implementation. After geometry optimization, the equilibration process is completed for the simulation box by using the Nose-Hoover thermostat. The initial temperature of the system is set as  $T_0=300$  K value for 1 ns. The achieved results of MD simulation for calculated temperature show that temperature changes occur as MD simulation time passes and reached the initial value after 1 ns. The equilibrium process has been done by monitoring temperature and potential energy, and the results have been captured in figure 2. It was observed that potential energy reached -489590 eV and -515358 eV values for MODEL 1 and MODEL 2, respectively. Finally, Radial Distribution Function (RDF) was calculated for the atomic matrix. Figure 3 shows our calculated results for this function. By comparing our calculated RDF with previous MD reports, we can say our computational settings in the current computational study are appropriate.

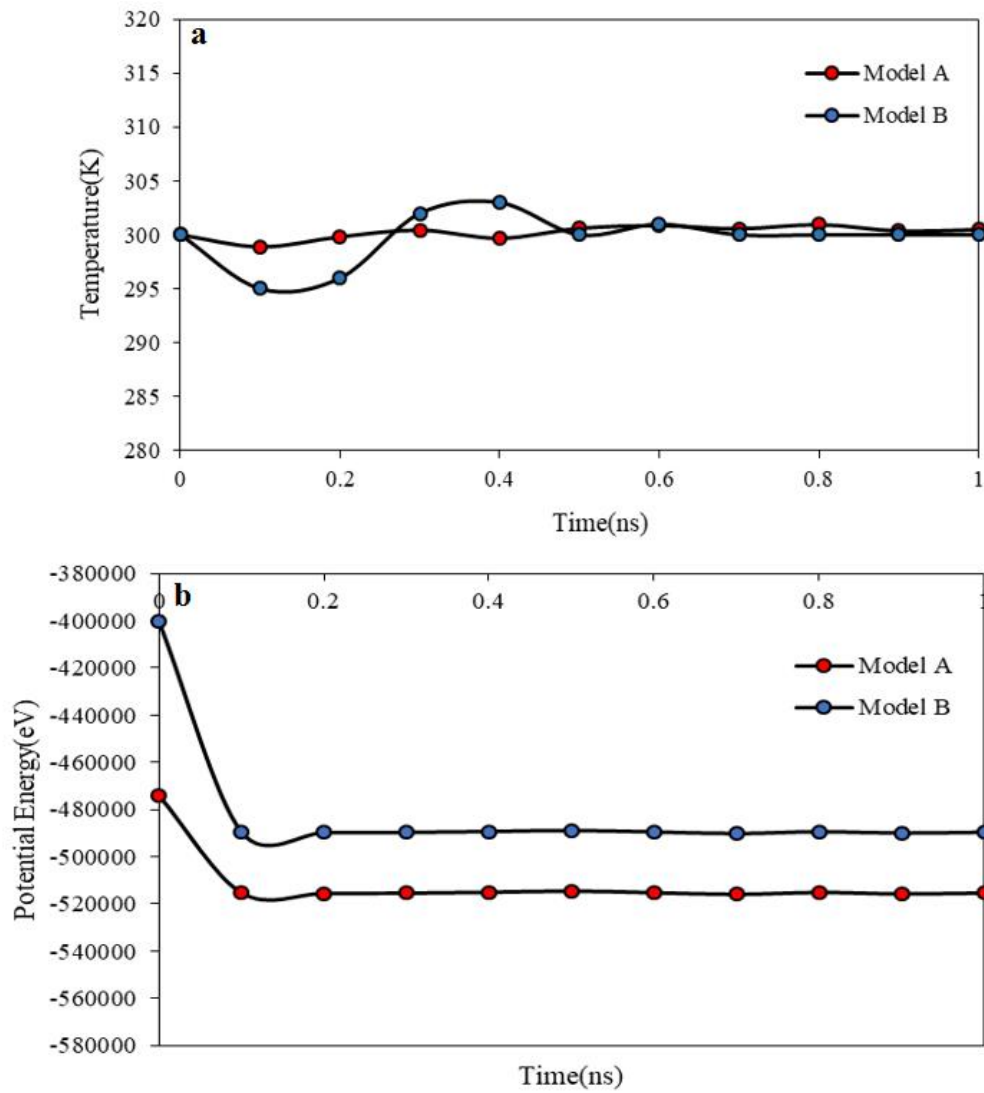


Figure 2. a) Temperature and b) potential energy variation of Ti-6Al-4V matrix-carbon steel system as a function of MD simulation time

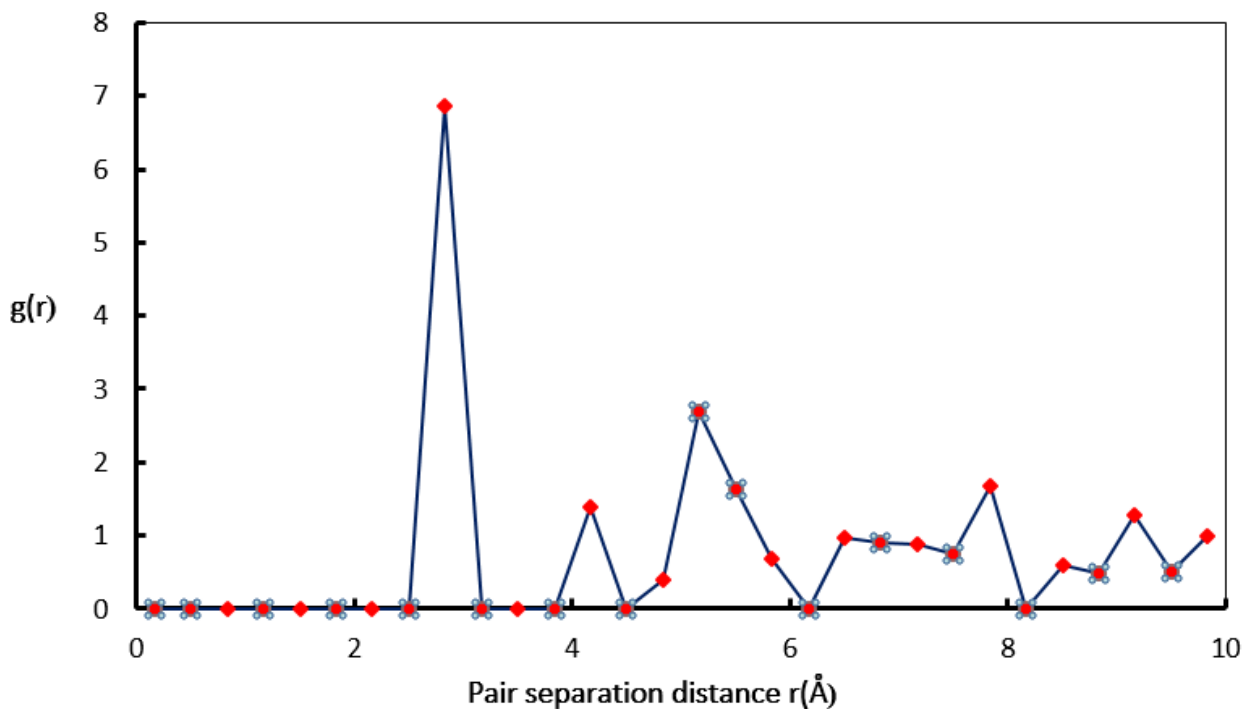


Figure 3. Radial Distribution Function (RDF) of pristine titanium sample as a function of used force-fields in the current computational study

### 3.2 Shot Peening Process Implementing to Simulated Structures

After equilibrium process detection in simulated structures, the shot peening process was done in our research depicted in figure 4. Also, the shot peening process was implemented in the Ti-based matrix. The described Models' properties in this step are listed in Table 5. Temperature variation of the atomic matrix after the described mechanical process is one of the important parameters for actual applications. Tables 4 and 5, shows maximum temperature variation as a function of the number of carbon steel particles and shot peening distance. The maximum temperature of the atoms simulated in the titanium surface layer is investigated. Computationally, the average temperature for each of the atoms in the titanium-based alloy surface layer is estimated. As reported in Table 6, MD simulation outputs show that, by increasing the number of carbon steel particles from 1 to 5, the maximum surface temperatures increased and reached from 380/383 K to 397/400 K values in MODEL1/MODEL2, respectively, this thermal behavior arises from atoms fluctuations increasing in simulated structures. On the other hand, as reported in Table 7, as shot peening distance increases, the maximum temperature calculated in this step decreases. By shot peening distance increasing to 15 Å, the maximum temperature reached from 416/ 425 K to 397/400 K. increasing particle distance from titanium surface caused decreasing in atomic force between particle and titanium surface and lead to decreasing maximum surface temperature.



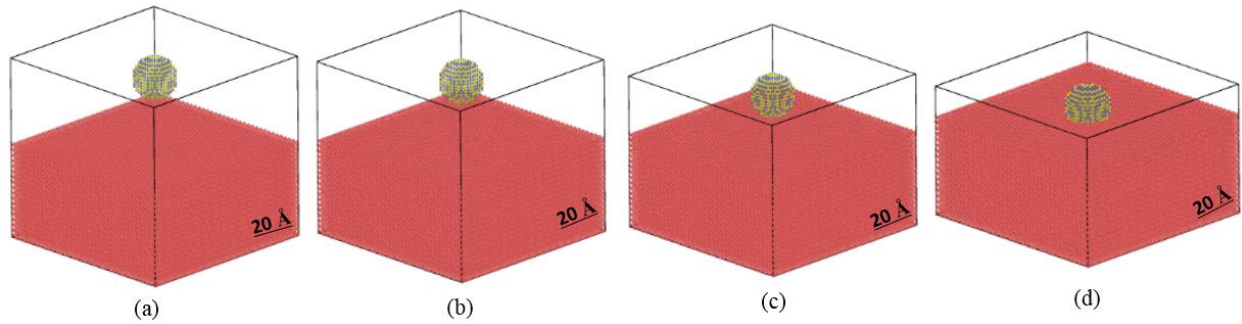


Figure 4. Arrangements of atoms in simulated structures during shot peening process at a) 1000000, b) 2500000, c) 5000000, and d) 10000000 time steps

Table 5. The diameter, velocity, number, and distance of carbon steel particles in the current computational study

Case Study No.	Diameter(Å)	Velocity(Å /fs)	Number of Particles	Distance(Å)
1	10	1	1	5
2	10	1	2	5
3	10	1	3	5
4	10	1	4	5
5	10	1	5	5
6	10	1	1	5
7	10	1	1	7
8	10	1	1	10
9	10	1	1	13
10	10	1	1	15

Table 6. Maximum values of alloy structure temperature after shot peening process as a function of carbon steel particles number

Numbers of Particles	Temperature (K)	
	Model 1 (LJ interaction)	Model 2 (EAM interaction)
1	380	383
2	382	386
3	388	390
4	391	395
5	397	400

Table 7. Maximum values of alloy structure temperature after shot peening process as a function of carbon steel particles number

Shot peening Distance(Å)	Temperature (K)	
	Model 1 (LJ interaction)	Model 2 (EAM interaction)
5	416	425
7	410	419
10	403	411
13	399	406
15	397	400

### 3.3 Surface compressive Residual stress

Residual stress is the stress that remains on the titanium surface due to plastic deformations after the shot peening process. We expected these physical parameter changes in simulated models by shot peening process properties changes. Figures 5 and 6 show residual stress changes as a function of the number of particles and shot peening distance. As depicted in figure 5, by increasing the number of carbon steel particles in the MD box, the residual stress increased. Particle number increasing caused residual stress reached from -413.2/-415.1 to -452.02/-456.97 MPa value in MODEL1/MODEL2. Also, as depicted in figure 6, by decreasing carbon steel particle distance from the titanium surface in the MD box, the mechanical behavior of the titanium surface layer was improved. So, by decreasing particle distance, the residual stress increased and reached from 413.2/414 to 419.63/422.28 MPa value in MODEL1/MODEL2.

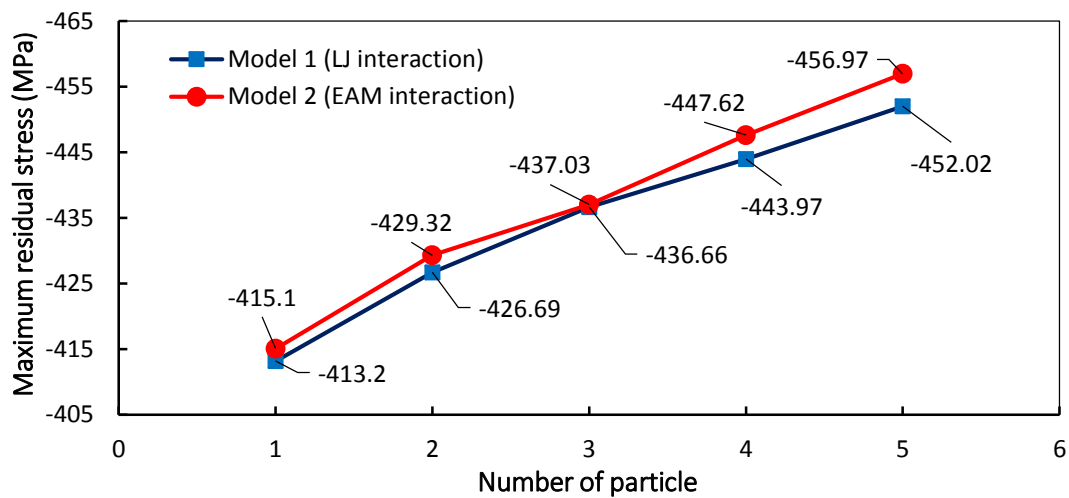


Figure 5. The maximum residual stress of Ti-based matrix after the shot peening process as a function of carbon steel particle number

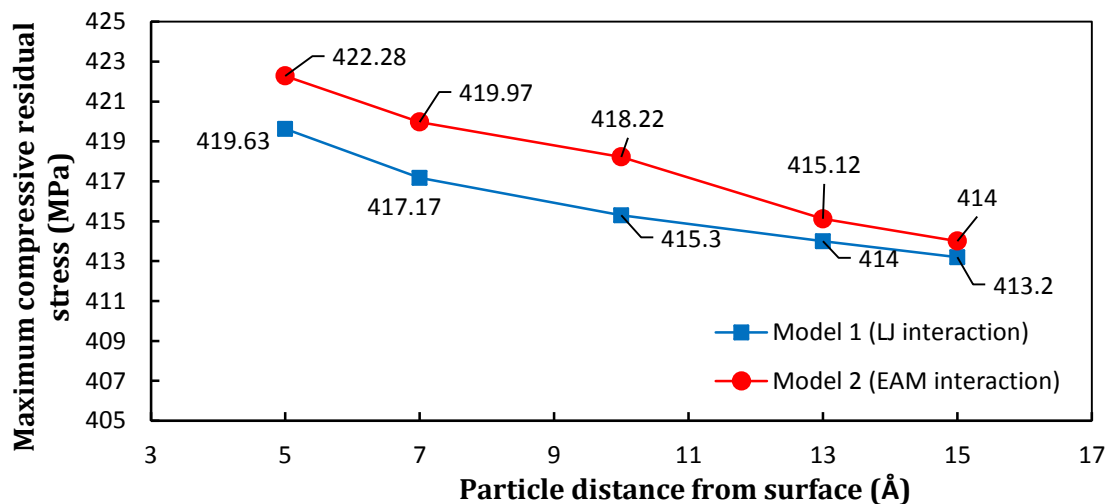


Figure 6. The maximum residual stress of Ti-based matrix after the shot peening process as a function of carbon steel particle distance

As reported before, the geometrical arrangement of atoms in pristine matrix changes after the shot peening process. Figure 7 indicated atoms arrangement changes in our MD simulations. Center of Mass (COM) is one appropriate parameter that can describe atomic arrangement variation in various atomic structures. This parameter of a distribution of mass in space is the unique point where the weighted relative position of the distributed mass sums to zero. In this step of our studies, we reported COM variation of the atomic matrix after the shot peening process. As listed in table 8, by particles number increasing from 1 to 5, the COM values increased from 0.015/0.012 Å to 0.035/0.032 Å in MODEL1/MODEL2, respectively. As listed in Table 9, by decreasing carbon steel particle distance from 15 Å to 5 Å, COM parameter in simulated structures increased from 0.023/0.018 Å to 0.015/0.012 Å in MODEL1/MODEL2, respectively. Physically, as distance decreases, the compression ratio of the alloy matrix increases, and the COM changes increase.

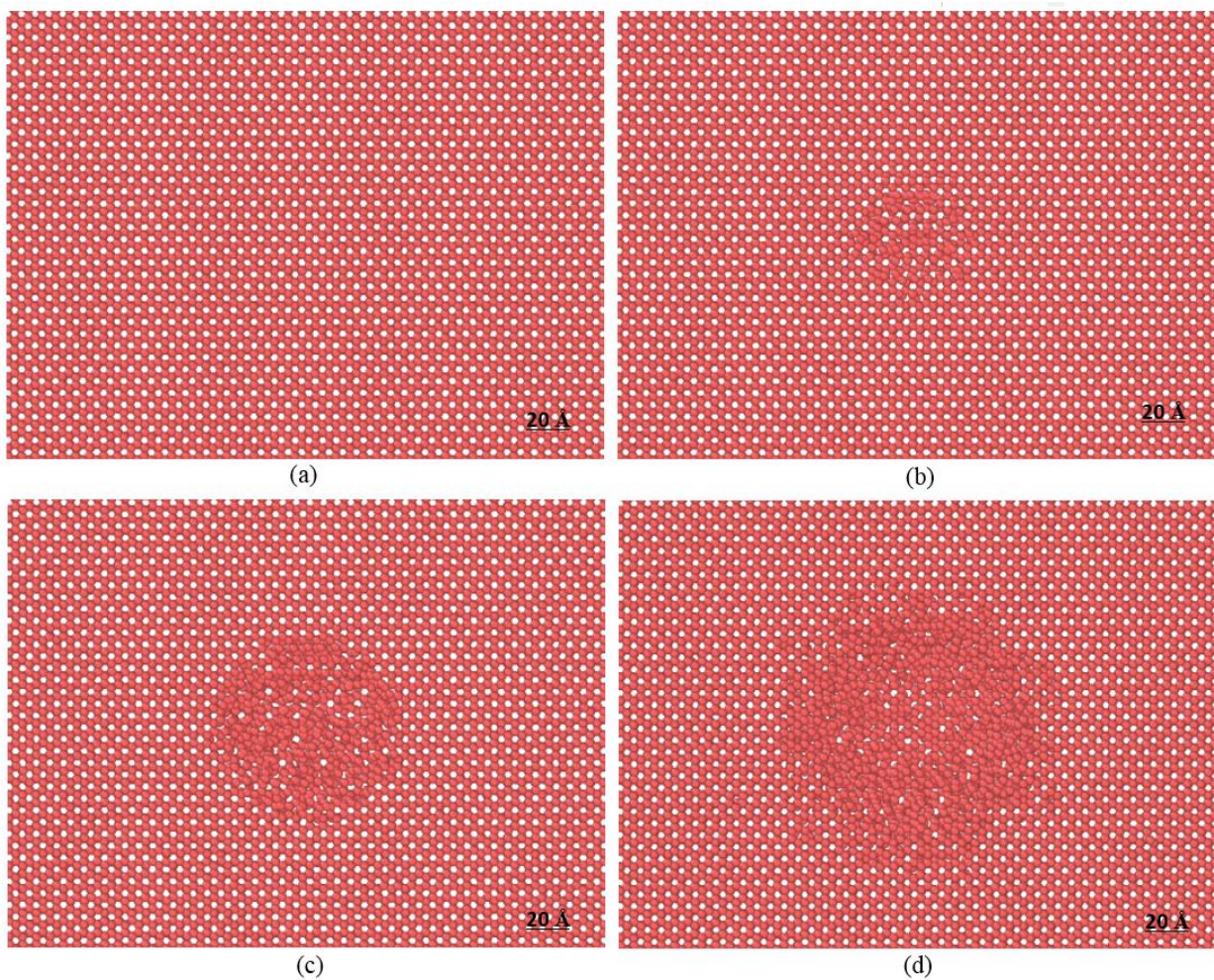


Figure 7. Atomic arrangement variation in shot peening process at a) 1000000, b) 2500000, c) 5000000, and d) 10000000 time steps

Table 8. The COM parameter of improved Ti-based matrix changes after the shot peening process as a function of carbon steel particle number

Numbers of Particles	Center of Mass Changes (Å)	
	Model 1 (LJ interaction)	Model 2 (EAM interaction)
1	0.015	0.012
2	0.018	0.016
3	0.022	0.018
4	0.027	0.024
5	0.035	0.032

Table 9. The COM parameter of improved Ti-based matrix changes after the shot peening process as a function of carbon steel particles distance

Shot peening Distance(Å)	Center of mass variation (Å)	
	Model 1 (LJ interaction)	Model 2 (EAM interaction)
5	0.023	0.018
7	0.021	0.016
10	0.020	0.014
13	0.017	0.013
15	0.015	0.012

### 3.4 Number of separated atoms

After the shot peening process, some Ti atoms were separated from the initial matrix surface. By carbon steel particles collision with alloy matrix surface, the inserted force from carbon steel particle to Ti atoms is bigger than the interatomic force between matrix particles. This procedure causes the separation of the Ti matrix after particles collide with them. As depicted in figure 8, the carbon steel number increasing caused an increase in the number of separated titanium atoms from the surface. Numerically, by using 5 particles in the shot peening process, the number of separated atoms reached from 18/15 to 24/21 atoms in MODEL1/MODEL2. As shown in figure 9, particle distance decreasing caused more titanium atoms fluctuations and led to an increase in the number of separated titanium atoms from the surface. The number of separated titanium atoms from the surface reached from 24/20 to 29/27 atoms in MODEL1/MODEL2 structure.

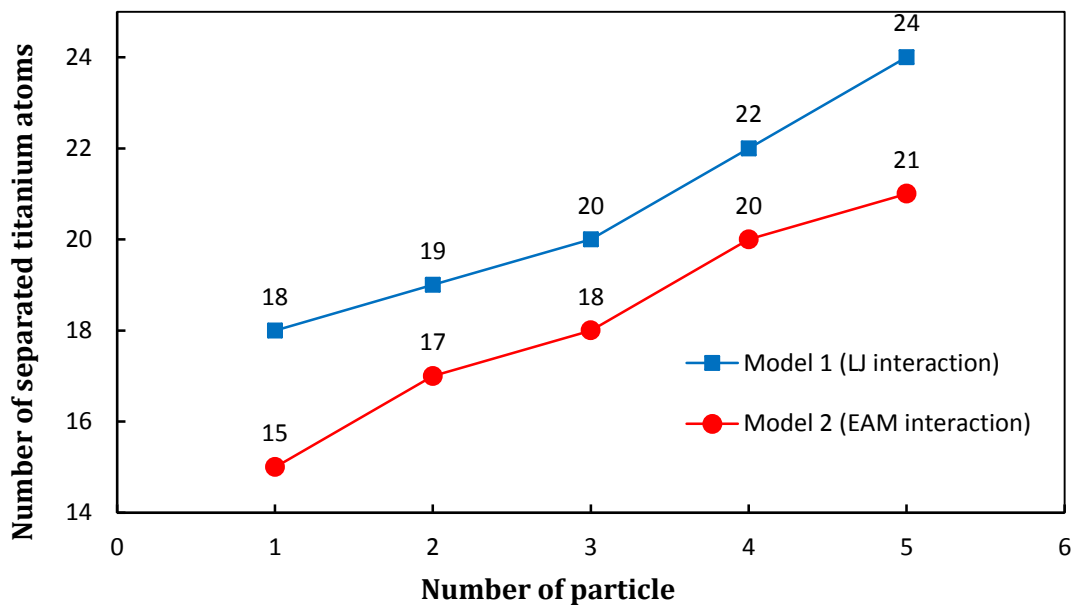


Figure 8. The number of separated Ti atoms forms a pristine matrix after the shot peening process as a function of carbon steel particle number

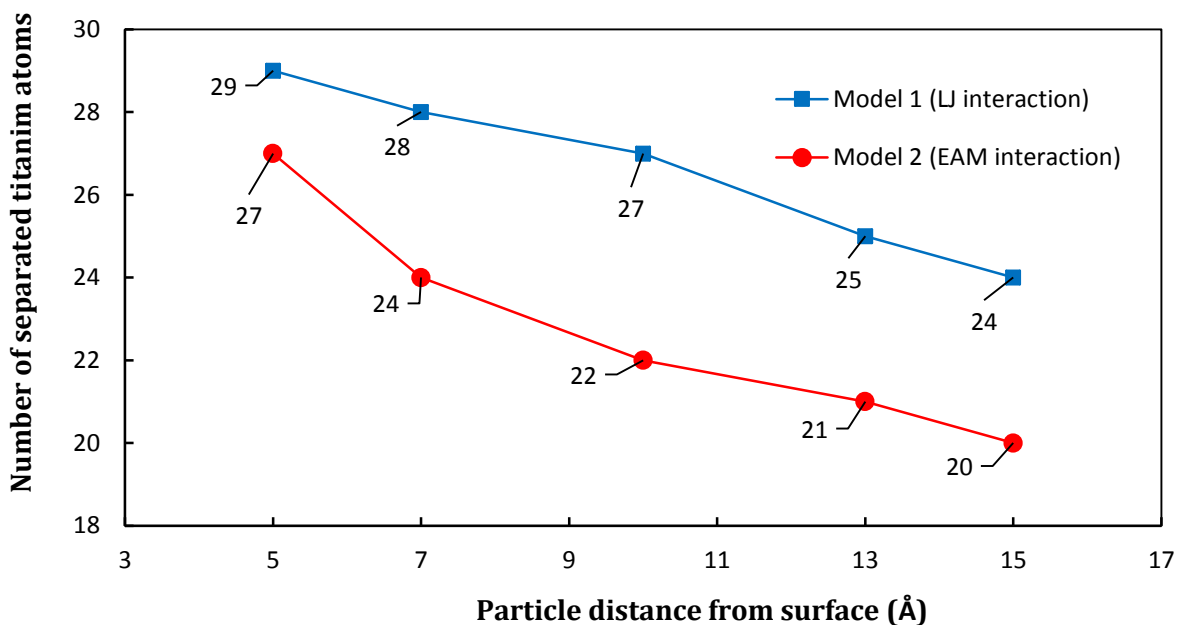


Figure 9. The number of separated Ti atoms forms a pristine matrix after the shot peening process as a function of carbon steel particle distance

### 3.5 Hardness of titanium surface

The Vickers hardness is another mechanical property that indicated the mechanical behavior of atomic compounds. In our MD simulations, this parameter is calculated by using the below equation:

$$V_H = \frac{2F \sin\left(\frac{136^\circ}{2}\right)}{d^2} \approx \frac{1.854A}{d^2} \quad (9)$$

Where,  $F$ ,  $d$ , and  $A$  are load, particle diameter, and the area of particle deposition within the atomic surface layer. This parameter variation is a function of the number of carbon steel particles and shot peening distance reported by the MD approach. Figures 10 and 11 show this parameter changes as a function of the number of particles and distances. From these figures, it can be observed that by increasing particles number, the mechanical behavior of the titanium surface layer was improved. The mechanical improvement caused increasing Vickers hardness values in the titanium surface layer. By using 5 particles in the shot peening process, the hardness value reached from 490.58/485.37 HV to 496.46/489.84 HV for MODEL1/MODEL2. In another hand, by decreasing particle distance, the mechanical behavior of the titanium surface layer was improved. Numerically, by particle distance decreasing to 5 Å, Vickers hardness value reached from 506.7/501.3 HV to 510.83/506.54 HV for MODEL1/MODEL2.

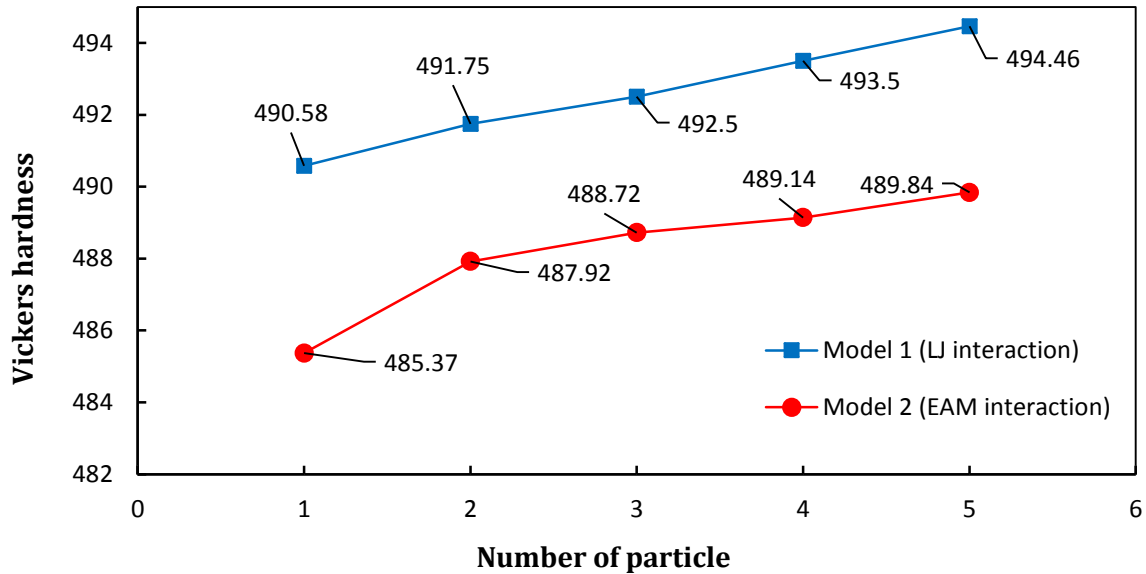


Figure 10. Vickers hardness of Ti-based matrix after shot peening process as a function of the number of carbon steel particles

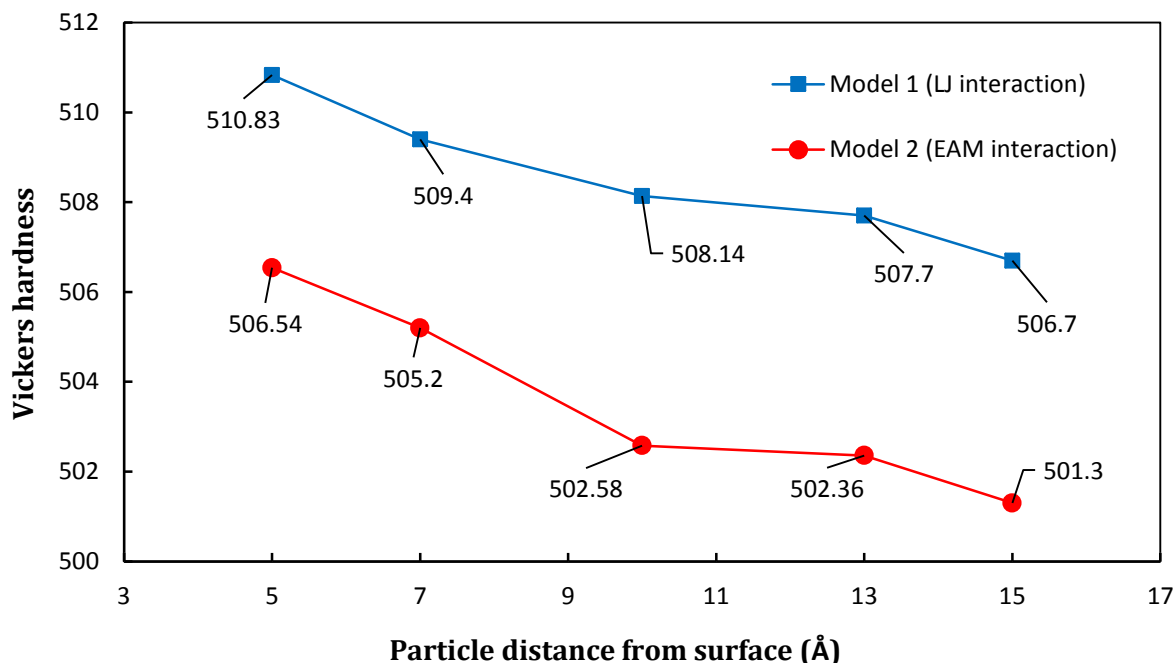


Figure 11. Vickers hardness of Ti-based matrix after shot peening process as a function of the distance of carbon steel particles

### 3.6 Roughness of titanium surface

The roughness of the Ti-6Al-4V alloy surface was calculated in the final step of our computational study. Carbon steel numbers increasing cause more atomic displacement in the titanium surface. By increasing atomic disruption, in the titanium surface, the roughness of them increased. Numerically, by using 5 number carbon steel particles in the shot peening process atomic roughness increased and reached 2.7/2.5 Å for MODEL1/MODEL2 as depicted in table 10. Also, by increasing carbon steel particles' distance from the surface, the atomic disruption increased and led to an increase in the titanium surface roughness, also the value of the titanium surface roughness reached 1.7/1.6 Å for MODEL1/MODEL2 as depicted in table 11.

Table 10. Roughness values of Ti-based alloy as a function of particle number in shot peening process

Numbers of Particles	Roughness Value of Alloy Surface (Å)	
	Model 1 (LJ interaction)	Model 2 (EAM interaction)
1	1.2	1.1
2	1.6	1.4
3	2	1.9
4	2.3	2.2
5	2.7	2.5

Table 11. Roughness values of Ti-based alloy as a function of particles distance in shot peening process

Shot peening Distance(Å)	Roughness Value of Alloy Surface (Å)	
	Model 1 (LJ interaction)	Model 2 (EAM interaction)
5	1.2	1
7	1.3	1.1
10	1.4	1.2
13	1.5	1.3
15	1.7	1.6

### 3.7 Comparison of MD results with experimental tests

In the study by Haghighi et al, the researchers showed that the hardness and wear resistance of the surface of AZ31 alloy increase in the shot peening process by using experimental tests [35]. In another study by Moradi et al, the researchers showed that the surface hardness of Ti-6Al-4V increased in the shot peening process by using experimental tests [36]. In another study by Maliwemu et al, the researchers showed that with increasing the distance of the shot particle from the surface of AISI 316L the surface hardness decreased and the surface roughness increased in the shot peening process by using experimental tests [37]. In another study by Iswanto et al, the researchers showed that by increasing the distance of the shot particle from 6 cm up to 12 cm on the surface of AISI 316L the surface hardness decreased, and the surface roughness increased in the shot peening process by using experimental tests [38]. The results of this study using MD simulations are in good agreement with these experimental studies.

## 4. Conclusions

In this computational research, we described the effect of particle number and distance from surface variations on the shot peening procedure. For this purpose, Molecular Dynamics (MD) simulation method was implemented by using the LAMMPS package. In simulated structures, Embedded Atom Model (EAM) and Lennard-Jones (LJ) force-fields used for atomic structures description. Technically, our computational study was done in two main steps. In the first step, the equilibrium phase of the Ti-6Al-4V alloy was described by temperature, potential energy, and Radial Distribution Function (RDF) parameters calculation. Next, the shot peening process was done in the MD box and the atomic behavior of the improvement surface layer was reported by various parameters such as maximum temperature, residual stress, the center of mass, departed atoms number, Vickers hardness, and roughness. MD results indicated temperature and potential energy of simulated structures reached 300 K and -515358 eV after 1 ns. This atomic behavior showed the equilibrium phase of the Ti-6Al-4V alloy matrix-carbon steel particle system. Furthermore, the calculations indicated an increasing number of particles and decreasing particle distance, improved mechanical behavior of titanium alloy, and led to increasing residual stress and hardness of titanium surface layer. Numerically, by decreasing particle distance from the surface, the values of titanium surface residual stress and Vickers hardness, and roughness increased and reached -419.63 MPa, 510.83 HV, and 1.7 Å, respectively in model 1. By increasing the number of particles, the values of titanium surface residual



stress and Vickers hardness, and roughness increased and reached 452.46 MPa, 494.46 HV, and 2.7 A in model 1.

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