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Research Paper

Effects of Colliding Particle Size and Velocity on Mechanical Properties of AZ31 after Surface Mechanical Attrition Treatment: Molecular Dynamics Simulation

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Abstract
In this study, the molecular dynamics method is used to simulate the SMAT process in the AZ31 workpiece. Molecular dynamics calculations in LAMMPS software have been used to investigate the effect of size, number, and velocity parameters of carbon steel particles on the mechanical and physical properties of the surface including residual stress, hardness, and surface roughness in AZ31 matrix has been investigated at the atomic scale. The simulation results during the SMAT process show that the residual stress in the AZ31 matrix increases with increasing the diameter of carbon steel particles and the particle velocity in the SMAT process has a significant effect on improving the mechanical properties of the simulated magnesium matrix. The highest residual stress and the largest increase in Vickers hardness in the SMAT process were calculated for the largest colliding particle. The maximum surface temperature of AZ31 decreases after SMAT with the increasing size of carbon steel particles. The results show that the roughness parameter increases with increasing colliding particle size.

Keywords
Molecular Dynamics Simulation, SMAT, AZ31, Mechanical Properties, Particle Size, Particle Velocity

1. Introduction

Hardness and smoothness are the most important mechanical properties of metal alloy surfaces. Surface Mechanical Attrition Treatment (SMAT) is one of the newest methods to increase surface properties [1]. In the SMAT process, the particles vibrate through a vibrating source and strike the surface of the workpiece in a random direction. This process creates a layer of nanocrystals on the surfaces of metal parts. The SMAT device has been shown schematically in Figure 1.

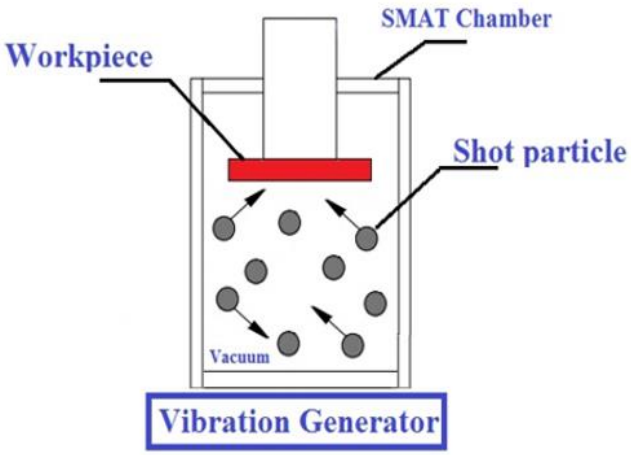

Figure 1. Schematic of the SMAT instrument

Many studies have been done on new surface modification processes or their simulation at the micro or nanoscale [2-6]. Considering the high cost of empirical experiments and the complexity of the SMAT process, numerical simulation methods have been used to investigate the effective parameters in this process. Molecular dynamics (MD) simulation is one of the most accurate methods for simulating engineering materials at the atomic scale [7-11]. Molecular dynamics has been successfully used by researchers for material modeling at the nanoscale or predicting the physical and mechanical properties in fluid mechanics or in new processes to surface modification [12-14]. This method has also been used to model materials in non-equilibrium conditions [15].

In a study, Rida et al. used the molecular dynamics method to simulate the products of the SMAT process [16]. The sample of the simulated material in this study was copper and they used the EAM potential function in their simulation. They tested the generated atomic sample under tensile stress with different strain rates and tried to make the strain rate comparable to the strain rate of the SMAT process. In this study, the effect of strain rate changes on yield stress is investigated and images of the atomic model under strain have been presented [16].

Zhang et al. in a study with numerical simulation by the Johnson-Cook method investigated the effect of the SMAT process on the surface of the AISI 304 matrix. According to the simulation results, the residual stress distribution was studied and the effect of impact frequency and bullet size on the compressive residual stress was investigated [17]. Among the studies conducted, Xilling and Wei provided a review to gather the latest advances in the modeling of material deformation processes leading to the formation of nanocrystalline structures in materials. In this study, the results of research in the field of molecular dynamics simulation of the deformation process with high strain rate and the collision of nanoparticles with the surface have been presented [18]. In another study by Yu et al., researchers investigated the effect of tensile deformation and fracture behavior on aluminum and lithium oxide alloys using molecular dynamic simulations [19]. In this work, the initial alloy sample was placed under an external force and its stress-strain diagram was calculated. According to the results, the relationship between grain size and strength was investigated. Moradi et al. investigated the effect of changing the velocity of spherical particles colliding with the surface in the Ti-6Al-4V peening process using molecular dynamics simulations [20]. In this study, two types of force fields, including the embedded atom method (EAM) and Lennard-Jones (LJ), were used to model colliding

atoms, with almost identical results. The effect of increasing residual surface stresses was observed with increasing velocity and particle size.

To the knowledge of the authors, few studies have been performed on SMAT simulations using molecular dynamics. This paper aims to investigate the effects of two main effective parameters on the mechanical and physical properties of the surface at the atomic level in the SMAT process with the help of molecular dynamics simulation results. The influence of the size and velocity of colliding particles on the mechanical and physical properties of the AZ31 surface such as hardness, residual stress, and roughness has been evaluated based on atomic results. The trend of the affected parameters due to variation of the variables can be used for investigation in practical applications.

2. Materials and methods

Magnesium has various alloy compounds with many applications in the industry due to their low density and good chemical and mechanical properties [21, 22]. AZ31 as the magnesium alloy contains 3% weight of aluminium (Al) and 1% weight of zinc. This material, like other magnesium alloys, has a hexagonal crystal structure.

Historically, the MD simulation approach was first developed in the field of theoretical physics in the 1950s. But today MD is used in various sciences such as physics, chemistry, drug delivery, biology, and mechanics [23-24]. In this research, the molecular dynamics method has been used to investigate the mechanical properties of the AZ31 matrix after the SMAT process. MD simulation was performed using LAMMPS software published by Sandia National Laboratories. In the molecular dynamics method, all calculations are performed according to Newton's equations, and in the simulation, the formulation of Newton's second law is used as follows: [25-26]:

$$F_i = m_i \frac{d^2 r_i}{dt^2} = m_i \frac{dv_i}{dt} \qquad (1)$$

In this equation, F_i represents the force applied to the *i*th particle with mass m_i. To integrate these equations the instantaneous forces applied to atoms must be determined. Then, by integrating the equation of motion, the trajectory of the particles, which describes the location, velocity, and acceleration of each particle, is determined over time, and thus the evolution of the trajectory over time will be known. In the next step, the average values of the properties can be determined using the trajectory. This method is algebraic and the state of the system can be predicted at any time by specifying the location and velocities of each atom.

In atomic calculations, the following equation has been used to determine the residual stresses of AZ31 atoms with the total volume of *V* [27]:

$$\sigma_{ij} = \frac{\sum_k^N m_k v_{ki} v_{kj}}{V} + \frac{\sum_k^{N'} r_{ki} f_{kj}}{V} \qquad (2)$$

Where, *m* and *v* are the mass and velocity of atoms, respectively. In addition, *f* and *r* are forces and distances between atoms. The indices *i, j,* and *k* represent the direction and number of atoms, respectively.

In these molecular simulations, for modeling the atomic interactions, the potential functions of EAM and Lenard-Jones have been used. The Leonard-Jones potential function with two repulsion and

attraction terms has been used to describe the interaction between the atoms of the AZ31 matrix and carbon steel particle. The EAM is used to express the interaction between the atoms in the metallic magnesium matrix. After defining the interatomic interactions, the time steps of the simulated structural structures are fixed at 0.01 ps, and the microcanonical and canonical ensembles are used for the process of balancing the atomic structures at the temperature of 300 K. MD simulation box lengths in the x and y directions are set to 50 nm and box size in the z-direction is set to 200 nm. Technically, in current MD simulations, the time step is set to 1 fs. Periodic boundary condition set to x and y directions and fixed one implemented to the z-direction. Also, canonical and micro-canonical ensembles are applied to the simulated atomic systems. In the canonical ensemble, three parameters of the system including temperature, volume, and the number of atoms are fixed through the simulation. In our MD study, the simulations were performed in the range of 10,000,000 to 20,000,000 time steps.

3. Results and Discussion

Molecular dynamics simulation of the SMAT process is performed for carbon steel particles with different diameters 1, 2, 3, 4, and 5 nm separately, and also in each part of the study, three consecutive collisions of particles are simulated separately. Figure 2 shows the atomic structure of the AZ31 and carbon steel particle simulation box and the collision steps of a particle with this workpiece.

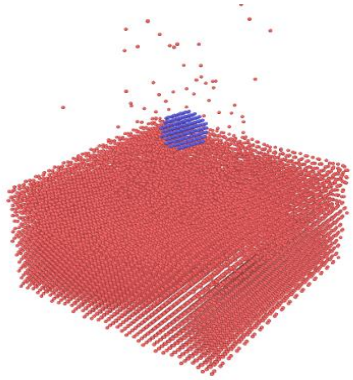

Figure 2. AZ31 molecular model at SMAT process

In the MD simulations, an AZ31 matrix inside the simulation box is first created, in which this atomic structure is bounded in all three directions by the box walls. After creating the atomic structure of the shot particles in this simulation box, the atomic model is equilibrated by the NVT ensemble at 300K. Figure 3 shows the total energy of the atomic structure during equilibrium in the NVT ensemble, which is related to the impact of a 1-nanometer particle on the workpiece. Based on this result, the total energy converged after 10,000,000 time steps and reached -33908 eV. The calculated results in this step were extracted from the log file of the LAMMPS computational package.

In the SMAT process, the great forces transfer from the particle to the AZ31 matrix at the collision area. This phenomenon increases the amount of residual stress on the surface atoms. The residual stress can be determined for all the atoms in the impact area based on equation (2). The maximum values of residual stresses of the atoms located at the collision region for different sizes of colliding particles were reported in Table 1. According to these residual stress values, as the size of the particles increases, the amount of residual stress which is applied to the matrix atoms rises. This is due to the

increase in collision energy at the contact area between the matrix atoms and carbon steel atoms. Numerically, the residual stress value for a 5 nm colliding particle after the first collision was calculated at 272 MPa, and this value was determined at 281 MPa after the third collision. On the other hand, the amount of residual stress after the second and third collisions gets larger than the first collision.

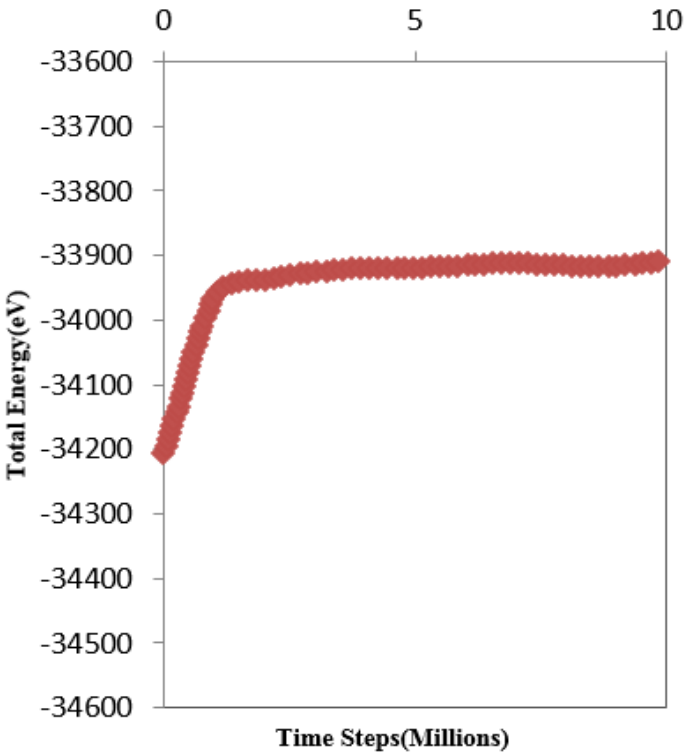

Figure 3. Total energy variation of the AZ31 atomic matrix and carbon steel particle as a function of MD simulation time steps

The effect of carbon steel particles' velocity variation on the residual stress of the simulated atomic structure is shown in Figure 4, based on the molecular dynamics simulations. As illustrated in Figure 4, as the particle velocity increased from 0.1 nm/ps to 0.5 nm/ps, the residual stress in the AZ31 matrix has been changed from 261 MPa to 272 MPa. According to the results, it is clear that as the velocity of the colliding particles increases, the interatomic forces and residual stresses caused by the collision increase. A similar trend in the increase in the residual stress values has been reported in reference [20] for the surface treatment process of titanium alloys.

During the impact of carbon steel particles on the surface of the AZ31 matrix, the atomic mobility of these atoms increases after the SMAT process. So, the temperature of the AZ31 atoms, which is a function of the velocity of the surface atoms, increases relative to the initial temperature. This increase in temperature at the collision surface atoms is greater than the underlying layer atoms.

Table 1. The maximum residual stress of AZ31 atoms as a function of particle size

Particle diameter (nm)	Residual stress (MPa)		
	1st Collision	2nd Collision	3rd Collision
1	261	263	268
2	264	267	269
3	266	270	272
4	269	273	277
5	272	276	281

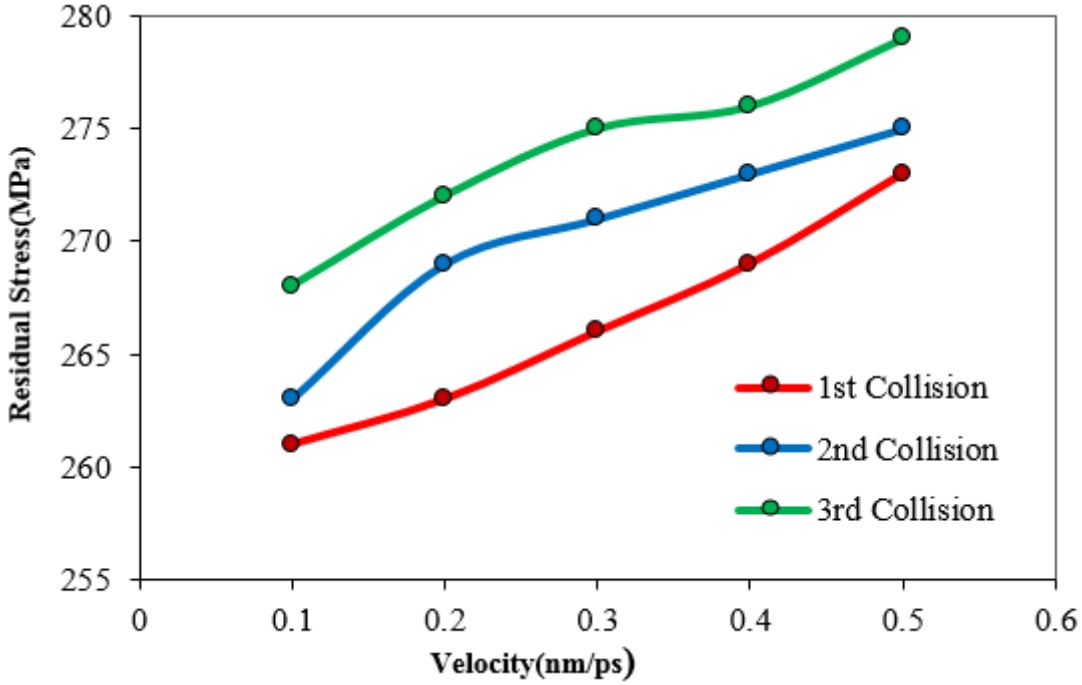

Figure. 4 The maximum residual stress of AZ31 atoms as a function of particle velocity

The maximum impact surface temperatures for different particle diameters after the third collision process is shown in Figure 5. Figure 5 shows by increasing the diameter of carbon steel particles, the maximum temperature in the atomic matrix slightly decreases. This phenomenon occurs because, with increasing particle size, the penetration depth of the carbon steel atoms in the AZ31 matrix increases, and the mobility of atoms decreases. As the diameter of the particle changes from 1 to 5 nm, the value of the temperature varies from 345K to 321K.

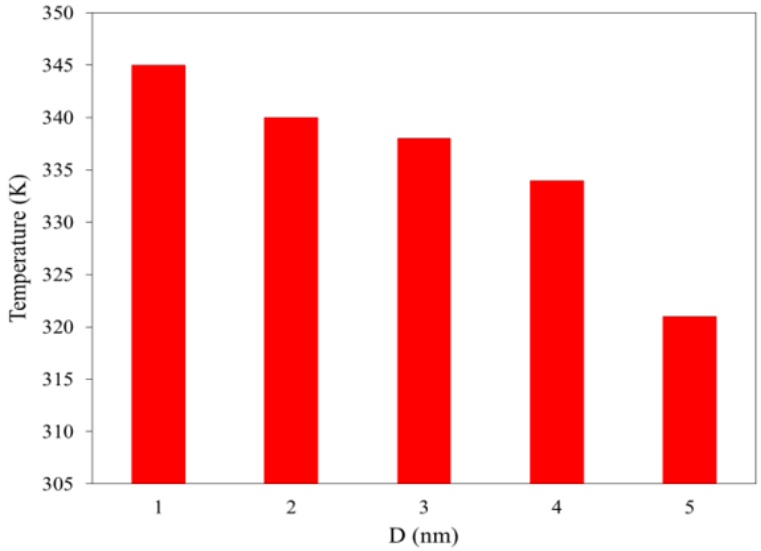

Figure 5. The maximum temperature of the AZ31 matrix after the third collision process as a function of colliding particle size

Hardness is one of the measurable mechanical properties which can be calculated after the simulation of the SMAT process. Atomically, the amount of this parameter increases gradually in the surface treatment process. The simulation results indicate a direct relationship between the size of the particle and the hardness of the atomic matrix. In this study, the hardness calculations were performed using the Vickers method. In this method, by calculating the load values, the diameter of the particle, and the amount of particle depth of penetration into the atomic matrix, the hardness of the atomic structures was calculated. The amount of calculated hardness in the atomic matrix increases with the increase in the number of atomic collisions. This atomic manner is due to the loss of space between matrix atoms in the simulated structures. Atomically, the SMAT process improves atomic arrangement in the simulated structures, which increases the hardness of the AZ31 structure.

In this study, the variation of the Vickers hardness parameter at the atomic scale was defined as the percentage of Vickers hardness increase in each collision compared to the Vickers hardness of AZ31in the first collision. Table 2 shows the obtained results of variation of Vickers hardness parameter based on atomistic simulation as a function of shot particle size. As can be seen in this table, the highest value of the increase in Vickers hardness during the SMAT process is achieved with the largest particle, and in most cases, the rate of increase in Vickers hardness decreases slightly with decreasing particle diameter. Also, Vickers hardness is affected by particle velocity variation. Based on the results of Figure 6, as the carbon steel particle velocity changes from 0.1 nm/ps to 0.5 nm/ps the Vickers hardness parameter changes from 5% to 25%. For all three stages of collisions, increasing the velocity of the particles increases the AZ31 hardness parameter. This phenomenon is due to the reduction of the atomic distance between the particles of the matrix after the collision and the increase of repulsive forces.

Table 2. Variation of Vickers hardness as a function of particle diameter

Particle diameter (nm)	Variation of Vickers Hardness (%)		
	1st Collision	2nd Collision	3rd Collision
1	5	13	14
2	9	14	17
3	11	16	18
4	13	18	20
5	16	21	23

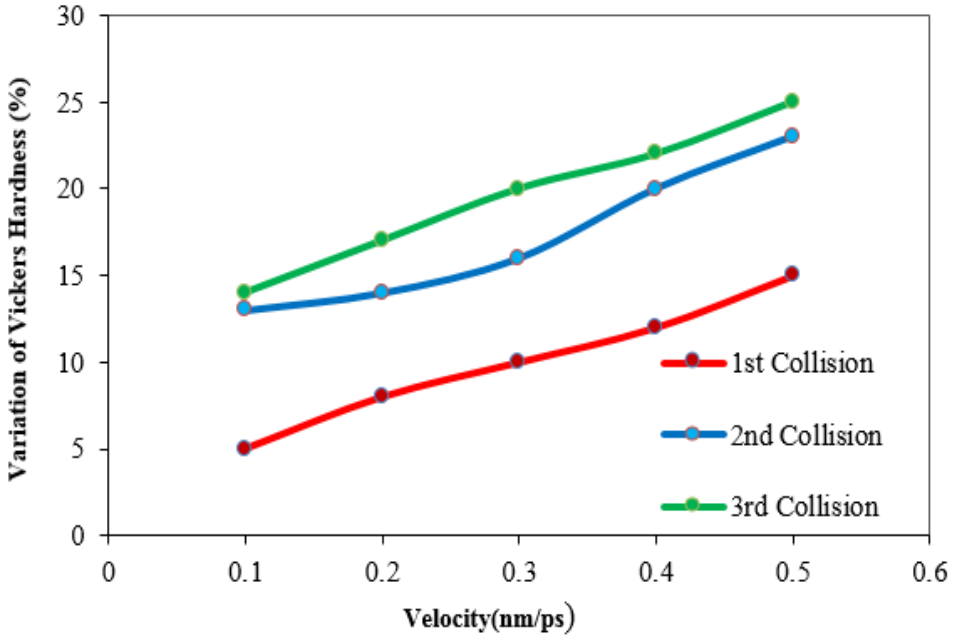

Figure 6. Variation of Vickers hardness parameter as a function of particle velocity

The roughness of the simulated atomic matrix is another improved physical factor after the SMAT process. Physically, we expect this mechanical parameter to be increased by the atomic collision phenomenon between the atomic matrix and the particles. On the other hand, to quantify the roughness of the AZ31 structure, the value of the matrix order parameter is calculated and reported. The roughness parameter increasing in atomic samples arises from the small crystal regions created in the simulated structure. From an atomic view, the regular arrangement of AZ31 particles causes more attraction force magnitude between them, and finally roughness of the pristine sample increases by the SMAT process. Physically, by these secondary crystalline region creations, the roughness of the simulated surface increases. According to Figure 7 results, the roughness value in the simulated AZ31 matrix increases with increasing particle diameter.

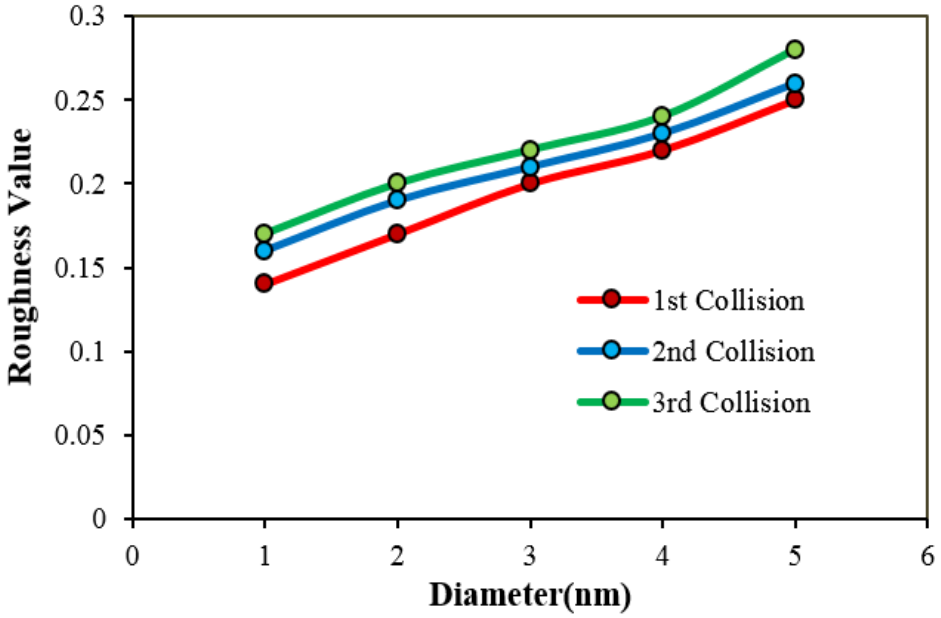

Figure 7. The roughness value of the AZ31 matrix as a function of particle size

4. Conclusions

The molecular dynamics method was used to study the SMAT process effects on the mechanical properties of the AZ31 sample. For this purpose, physical parameters such as maximum temperature, residual stress, Vickers hardness, and atomic roughness were calculated in the simulated AZ31 matrix. The atomic simulation of the SMAT process was performed by using 5 various particle sizes. Technically, in the molecular dynamics simulations, three continuous collisions occurred. The simulation results showed the following conclusions: There was an inverse relationship between the maximum amount of temperature and the particle size. By particle size increasing to 5 nm in the first collision, the maximum temperature of the AZ31 matrix decreased to 376 K.

The residual stress of the AZ31 matrix increased with particle size and number of collisions in the SMAT process so the amount of residual stress in the atomic structures increased to 281 MPa for the third collision of a 5 nm particle. Furthermore, with carbon steel particles increasing, the residual stress of the matrix converged to 272 MPa. The Vickers hardness in the simulated AZ31 matrix increased with the size and number of particles. The highest rate of increase in Vickers hardness during the SMAT process was achieved with the largest particle. The amount of roughness in the atomic matrix can be expressed using the order parameter in molecular dynamic simulations. MD results indicated, the roughness parameter increased by enlarging the particle size and velocity. The trend of variation of mechanical and physical surface properties in terms of effective parameters in the SMAT process, which was obtained based on the results of molecular dynamics, can be used in practical experiments and reduce the cost of trial and error. Moreover, molecular dynamics can be used for modeling the surface treatment of other industrial alloys.

5. References

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