

Abstract

Application of indentation and scratch tests of one and two layer coatings on a substrate were modeled by LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). To be realistic, materials and lattice of the coatings and substrate were chosen different. In the solutions, the load as displacement for indentation and scratch were defined with variable command in LAMMPS and was applied in loop-next. In addition, the model used in the solution was created in 3D. Atomic distributions before and after scratching were obtained by VMD tool. Also forces were given as a function of MD timesteps.

Introduction

Surface coatings from nanometers to several hundred micrometers are an important approach to changing surface properties for the requirements of a given application. They are widely used in major industrial areas including sensors, energy saving coatings for solar devices, absorbers/reflectors/emitters, cutting and forming tools, protective environment-resistant or decorative coatings, and information storage and micro-electronic devices. Surface coatings modified by ion or laser treatment will also be of great importance to the future of industrial technology. It is very important to know coating behavior in advance under working conditions, so that designs can be done safely. Because if a coating fails its function may be deteriorated. In coated systems, bonding properties of coating to substrate play a crucial role in the reliability of products to which they are applied. An obvious way to understand coating behavior is to apply indentation and scratch tests on nanoscale. These techniques are widely used for understanding coating behavior and obtained mechanical properties of thin coating. Nanoindentation is a kind of indentation hardness tests applied to small volumes. It is maybe the most commonly applied means of testing the mechanical properties of materials. The nanoindentation method was described in the 1970s to measure the hardness of small volumes of different materials. Scratch tests used to be applied on a macroscopic, microscopic, and nanoscopic scale, the latter with the atomic force microscope (AFM). The most recently emerging development is nanoscratching, using nanoindenters equipped with a two-dimensional (2D) or three-dimensional (3D) transducer. Scratching of surfaces is closely related to the field of tribology, but greasing is to be avoided for original materials characterization [1]. Nanoindentation and nanoscratching systems are generally used to investigate the properties of materials at small scale, such as, friction, hardness, resistance, etc... To design these systems are very difficult by experiments because nanoscratching involves changes in only a few atomic layers at the surface region. So MD (Molecular Dynamics) has become an important tool in the study of scratching in nanoscale. Many researchers used MD simulations to make indentation and scratch tests for different materials' atoms. Shimizu et al. performed a two-dimensional MD simulation model to investigate the nano-scale stick-slip phenomenon which is commonly observed in the surface measurement using an AFM [2]. Fang et al. presented a three-dimensional MD model [3] to study the tool geometry and processing resistance effect on AFM-based cutting process and they applied this model on gold and platinum thin films [4]. The scratching behaviors of nickel and iron surfaces by MD simulations for different indenter shapes were investigated [5, 6]. Kun et al investigated the atomic scale tribological behaviors nano-grained and single crystal copper system using MD simulations [7]. There are many valuable studies on nanoscratching and nanoindentation by MD simulations in the literature [8-12].

In this study, application of indentation and scratch tests of two layer coatings on a substrate were modeled by Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) developed by Sandia National Laboratories.

Materials and Methods

3D simulations performed for aluminum atoms coated with copper atoms. Dimension of orthogonal simulation box is from (0 -40.5 -4.05) to (405 40.5 4.05) with angstrom unit. 17257 atoms were created in this box by copper and aluminum FCC lattices. Periodic boundary conditions were applied in the z-direction. LAMMPS metal units were used. Cu-Cu, Cu-Al and Al-Al atomic interactions were described EAM alloy potential parameters (Embedded Atom Model). Boundary atoms, thermostat atoms and Newtonian atoms were described as different atom types of Al. And then Al and Cu coating was applied. A rigid spherical indenter was modeled as $R=6.0A^0$. Scratching was applied with looping. For this, a variable called i was written to 1000 and scratching process was continued with $0.05A^0$, $0.10A^0$, $0.15A^0$ and $0.20A^0$ steps. Depth of indenter in the atoms was chosen as $5.5A^0$. Energy minimization was applied. In the nanoscratching processes, the rigid indenter is moved for different four steps meaning different four speeds along the x direction. The boundary atoms are held fixed to prevent the system from translating during the processes. Heat dissipation is carried out by keeping the thermostat atoms at a constant temperature of 293 K by velocity scaling method at every time step. Simulation results were evaluated by VMD visualization tool [13] and GNUPLOT softwares.

Results and Discussion

The aim of the present study is to obtain the behavior of the interface between substrate and coating. To show this, the forces of the interface at x-direction for each four scratching steps. Firstly, the initial configuration of Al and Cu atoms is shown in Fig.1. In this figure, there are three different regions as colored with purple (Cu coating atoms), blue (Al coating atoms) and ochre (other all of Al atoms). Also the starting point of the indentation and the scratching processes was marked. Fig.2, Fig.3, Fig.4 and Fig.5 show the states of system after indentation and scratching processes at 0.05, 0.10, 0.15 and 0.20 scratching steps, respectively. As can be seen in these figures, the scratch distance at x-directions increases with increasing scratching steps because of the same solution times. Forces at x-direction for interface between substrate and coating regions were calculated for each scratching steps by using *compute group/group* command. These force curves as a function of MD timesteps can be seen in Fig.6.

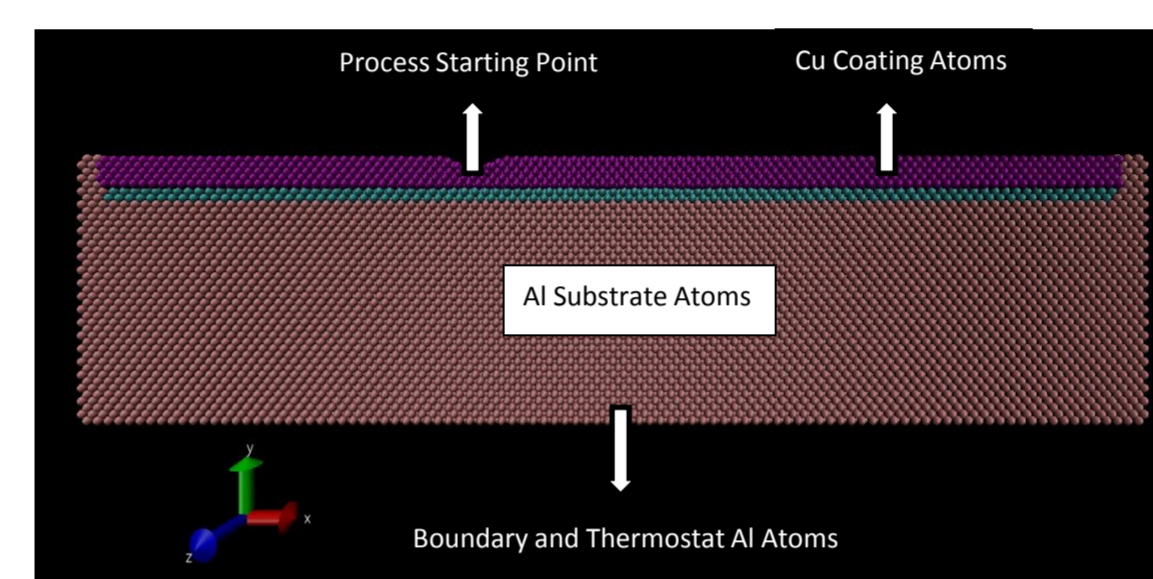


Fig.1. Visualization of initial state of atoms

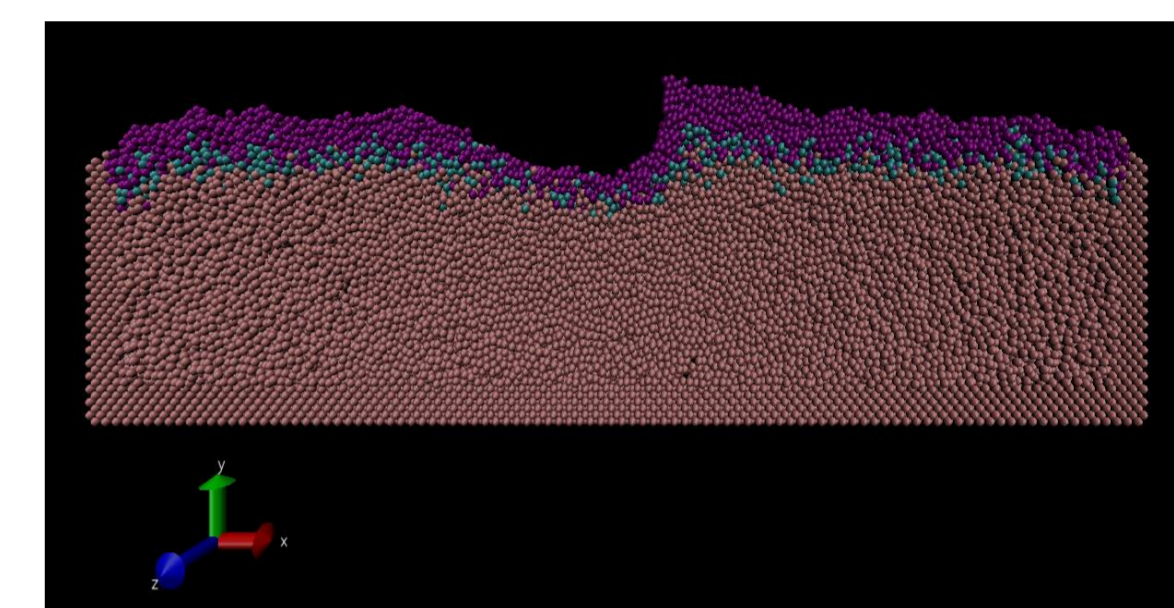


Fig.2. State of system at 0.05 scratching step

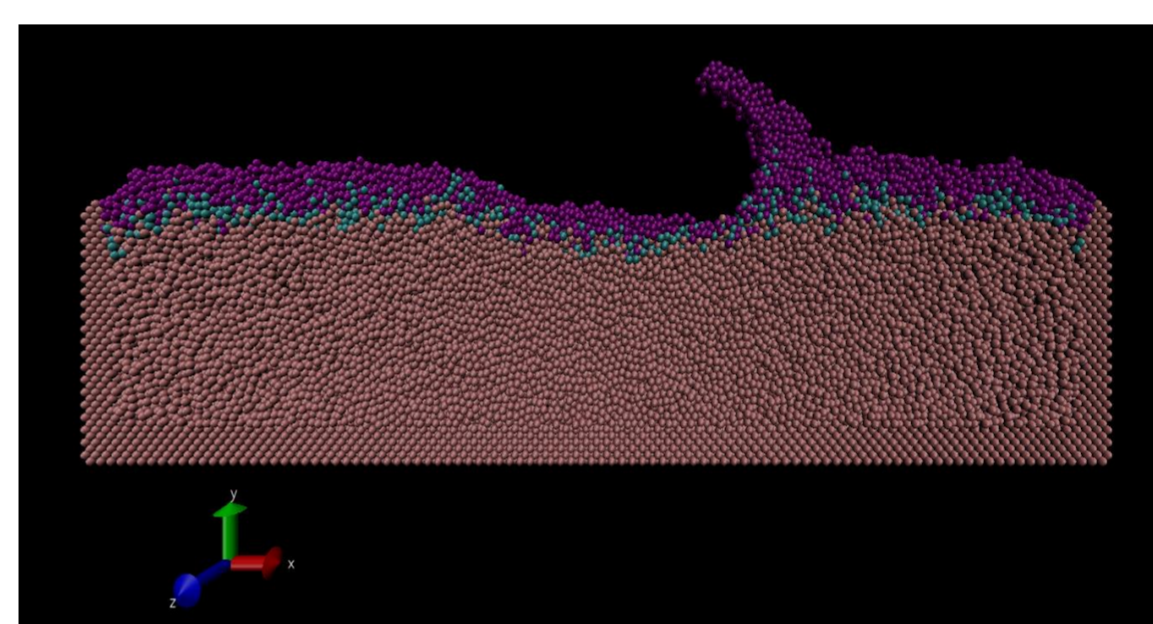


Fig.3. State of system at 0.10 scratching step

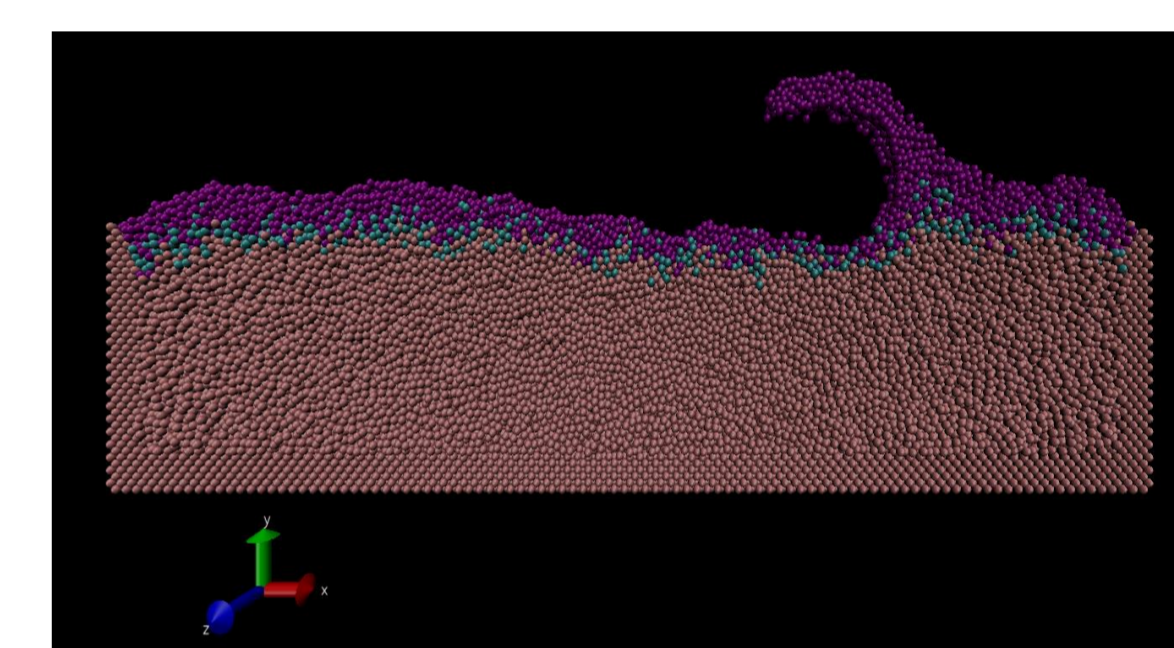


Fig.4. State of system at 0.15 scratching step

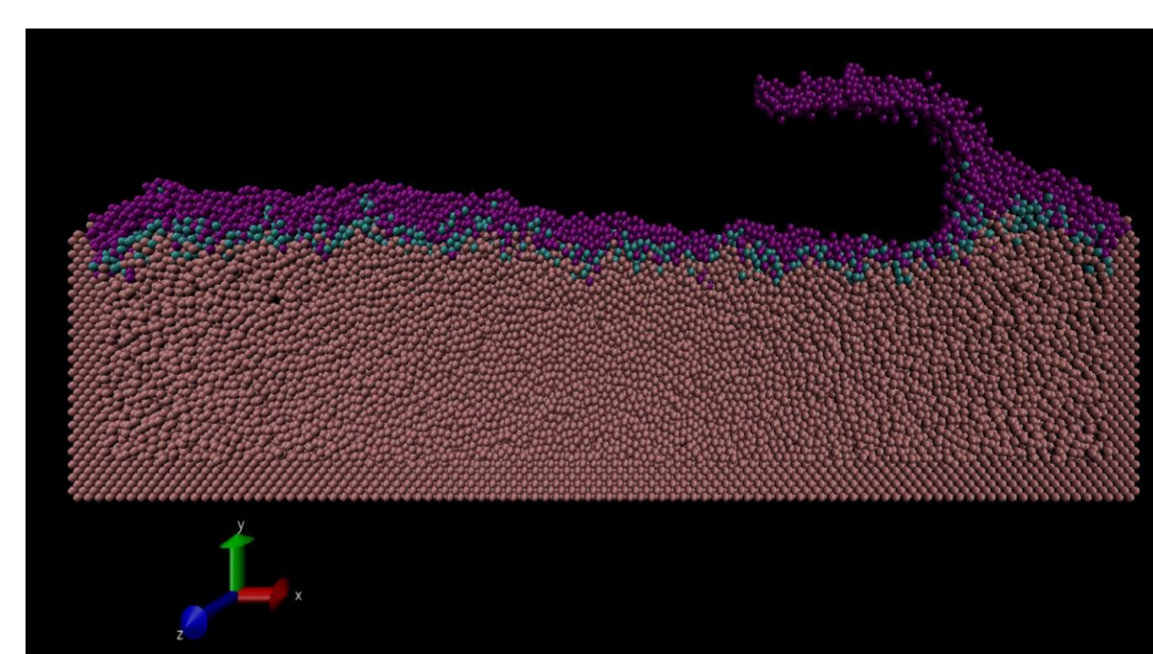


Fig.5. State of system at 0.20 scratching step

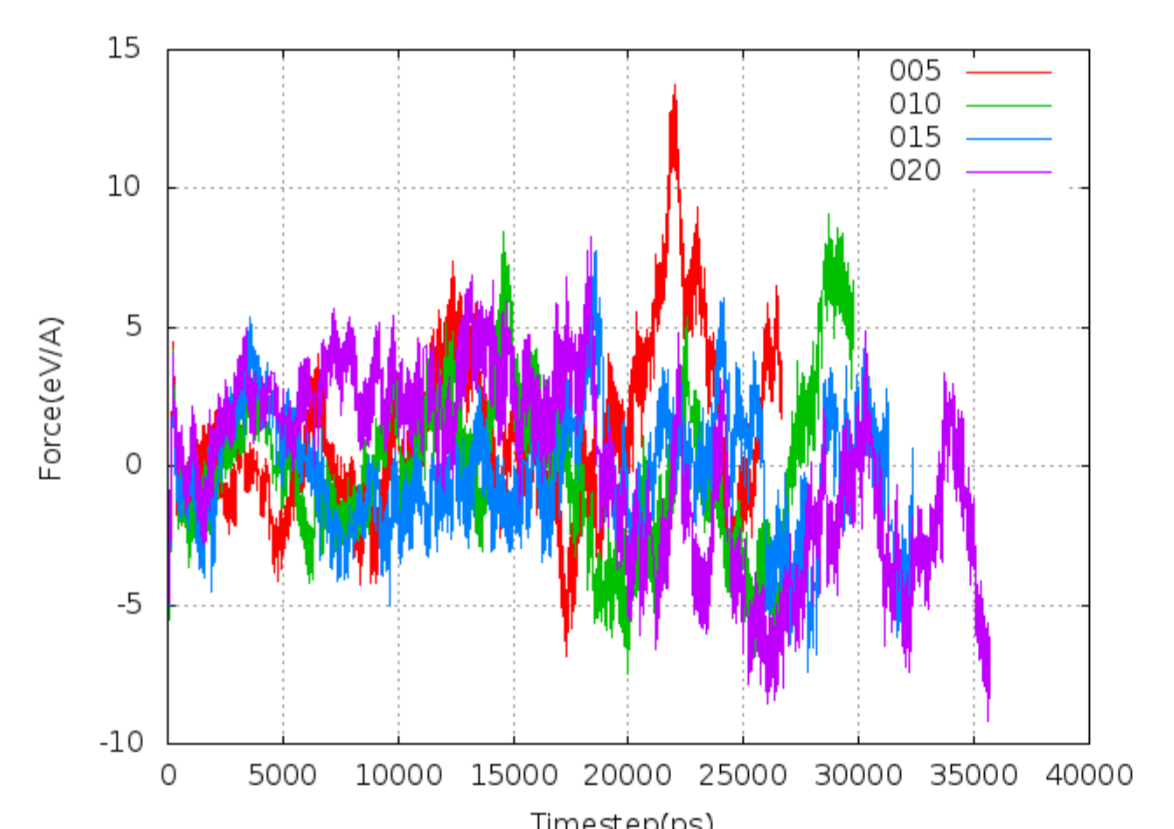


Fig.5. Forces at x-direction

Conclusion

Modeling of indentation and scratch technique with LAMMPS is offered in this presentation. We are enriched this model by two different coating. As a results, this model can be used in the future nano-applications such as nanomachining, tribological characterization of materials, estimating mechanical properties of coated samples etc...

References

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