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Atomic Simulation of Temperature Effect on the Mechanical Properties of Thin Films

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ABSTRACT

The molecular dynamic technique was used to simulate the nano-indentation test on the thin films of silver, titanium, aluminum and copper which were coated on the silicone substrate. The mechanical properties of the selected thin films were studied in terms of the temperature. The temperature was changed from 193 K to 793 K with an increment of 100 K. To investigate the effect of temperature on the mechanical properties, two different ways including step by step and continuous ways, were used. The temperature in the indentation region was controlled and the effect of temperature increase due to the friction between the indenter and the film was taken into account. The temperature effects on the material structure, piling-up and sinking-in phenomena were also considered. The results show that the elasticity modulus and hardness of thin films decrease by increasing temperature. These mechanical properties also decreased due to the increase in temperature, in the indentation region, which in turn was due to the interaction between the indenter and the thin film.

1. Introduction

Thin films have been extensively used in various engineering applications such as semiconductors, storage systems, lens coatings and micro-electromechanical systems (MEMS) to improve their performance [1-3]. Metallic thin layers such as aluminum, copper and gold which are coated on hard substrate such as silicone and germanium are of great importance in semiconductors and micro-electronic systems. Mechanical properties of these thin films which are different from their bulk samples, should be determined precisely for trustful performance of these micro-equipment [4, 5]. As the thickness of these thin films in industrial applications becomes thinner, measuring their mechanical properties becomes more and more difficult. So, the traditional ways used for bulk materials are not appropriate for thin films [6]. Environmental circumstances of such films such as the temperature and the moisture have also great effects on their mechanical behavior [7].

Few techniques exist for determining the mechanical properties of thin films, among which the nano-indentation experiment has received more attention in recent years. In this method, the main aim is the measurement of hardness and elasticity (Young's) modulus of different materials. Many researchers have used the theoretical and experimental methods to extract the mechanical properties of coatings from the film-substrate systems in the nano-indentation [8-12]. As the nano-indentation equipment has some limitations such as tip rounding effects, machine resolution and signal-to-noise ratio, extracting meaningful experimental results from the indentation depths less than 10 nm is relatively difficult [13, 14]. In the experimental studies, it is common to limit the indentation depth to a small fraction, typically 10%, of the film thickness to avoid substrate effects on the measured properties. This restriction becomes increasingly problematic when the film thickness is so small that

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10% of the film thickness falls in a range where the effects of indentation size and surface roughness can complicate the results. Therefore, finding new methods for determining the mechanical properties of the thin films over a wide range of indentation depths that are insensitive to the physical parameters such as surface roughness and pile-up/sink-in is important [15].

Atomistic simulations such as Molecular Dynamics (MD), which is a methodology for a detailed modeling of materials at atomic scale, have provided beneficial information about the atomic structure, subsurface deformations and dynamics of defects within the material. In the MD technique, the motions of individual atoms/molecules in the models of materials are computed and the way their positions, velocities and orientations changes with time is described. Therefore, MD simulations have been widely used to study the nano-indentation and explore the contact and friction mechanisms at nanoscale [16-18]. Recently, several researchers have applied MD models to nano-indentation experiment for investigating the mechanical properties of thin films. For examples, Shi and Falk applied MD models to simulate the nano-indentation process for crystalline and metallic thin films and to study the structural transformation and atoms localization during the indentation [19]. Peng et al. used the MD simulation for a 3 dimensional model of nano-indentation test for the aluminium coating on the silicone substrate [20]. Hwang et al. simulated the copper cluster deposition on the silicone substrate using the molecular dynamics approach [21].

The main objective of this study is to investigate the effect of temperature change on the hardness and elastic modulus of selected thin films coated on the silicone substrate using MD simulation of nano-indentation process. To simulate this procedure, 3-dimensional models of samples are created using the open code software for molecular dynamics simulation, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). To define the interactions between the atoms, the hybrid interatomic potentials are used. The Morse potential is applied for describing the interaction between the metallic atoms, and the Tersoff potential is employed for modelling the interaction between the silicon atoms. Two simulation approaches are used to control the local temperature of the indentation region. Considering the load-displacement curves obtained from the simulation, the mechanical properties of metallic coating are determined. As the changing and controlling the temperature in the nano-indentation experiment, specially for temperatures beyond 100°C that are very difficult and costly, the use of MD simulation for studying the effect of temperature on the mechanical properties of materials can be appropriate.

2. Modelling Details

In this study, the mechanical behavior of a range of single crystal metals i.e. aluminum, titanium, copper and silver, is investigated by modelling the nano-indentation process. As it is shown in Fig. 1, the MD models simulated in this study consist of a conical diamond indenter tip, a silicone substrate and a thin film coated on the substrate. Thin film coatings of copper, aluminum and silver have FCC structures and thin film coatings of titanium have a HCP structure, which are oriented in the plane (1 0 0). These coatings are placed on a substrate of silicon oriented in the [1 0 0] direction.

The conical indenter tip has a half-angle of 70.3° and is made of 24818 diamond atoms of single crystal diamond structure, which has a lattice parameter of 5.43 Å and the tip radius of 1 nm. The indenter tip is supposed to behave as a rigid tip, therefore, its shape does not change during the indentation process.

The Morse interatomic potential used to define the interaction between the metallic atoms can be written as the following:

$$V(r)=D\left[e^{-2\alpha(r-r_0)}-2e^{-\alpha(r-r_0)}\right] \quad (1)$$

where $V(r)$ is the potential energy function, r is the interatomic distance between atoms i and j, and D, α, and r_0 indicate the cohesive energy, elasticity modulus, and equilibrium distance, respectively. The Lorentz-Berteloth rules are used to apply the Morse potential for the interatomic potential between metals and Silicon atoms. There are several parameters that should be specified for different atomic species interactions in the Morse function. For calculating these parameters, the Lorentz-Berteloth rules are employed [22].

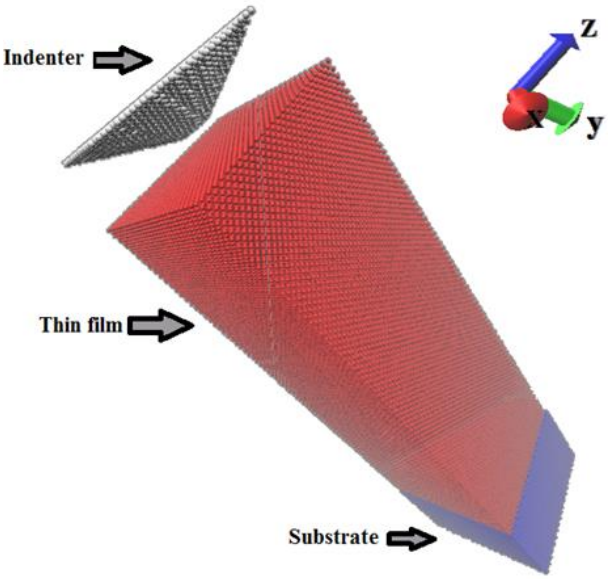

Figure 1. The MD simulation model

Parameters of the Morse potential for the selected metals are obtained from studies, done by Yan et al. [23] and Fang et al. [24]. The Tersoff potential function is applied for silicone substrate [25].

The dimensions of the thin film and substrate in the x and z directions are about 10 nm×10 nm, and the thickness of the substrate is about 20 nm. The thickness of the layer in the y direction, is supposed to be 100 nm according to the results presented in the study, done by Ayatollahi et al. [26]. The indenter moves only in the y direction. Across the lateral planes of the model, (in the x and z directions) the periodic boundary condition is used. In the y direction, the top surface of the coating which is in contact with the indenter is set to be free but the bottom plane of the substrate is fixed to avoid the movement of the model due to the indenter force. After each set of 100 time steps, the temperature and velocity of particles are rescaled according to the initial temperature up to the end of the process. In this modelling, the time integration of Newton motion equations is used by applying the velocity Verlet algorithm with a time step of 1 fs.

In the initial model, the atoms stand in the ideal crystalline structure without any movement. Therefore, in the first step of simulation, the sample is allowed to reach equilibration according to the initial temperature. In this simulation, the initial velocities are randomly selected and they are such set to indicate the total zero momentum and temperature of the model. These velocities change during the simulation. For determining the appropriate time step, as an important parameter, it should be noticed that smaller time steps lead to more accurate results but they also need more steps to perform the simulation process resulting in higher computational costs. Large time steps may also generate numerical instability. Therefore, for avoiding these errors, the time step that is conventionally applied in the molecular dynamics is in the order of fs. The time step considered in this study is 1 fs.

At the beginning of the simulation, for avoiding an interaction between the indenter and specimen, the indenter tip is positioned above the top surface of the specimen at the distance of one inter atomic cutoff radius. The indenter is inserted into the free surface of the coating using the displacement control method at a constant speed. The indentation speed is considered to be 50 m/s, to have a reasonable computational time in the simulation. This speed is relatively high in a real indentation experiment, but since the indentation speed has no effect on the main features of atomic rearrangements in the MD simulation, it can be applied for the MD modelling of this procedure [20]. The maximum indentation depth is set to be about 1.6 nm. As the presence of the surface roughness in the sample and imperfect geometry of the indenter tip are unavoidable in the real experiments, the maximum indentation depth is more than that of the MD simulation [27].

The indenter is held for about 10 ps at the maximum depth to allow the model for re-equilibration. Then, the indenter is removed at the same speed as the loading continues until it has no interaction with the surface of the thin film.

In the MD simulation, the temperature is computed as the kinetic energy divided by a number of degrees of freedom. For controlling the temperature of particles in the MD simulation, thermostatting command is applied. Two types of thermostats are used in this study. First, the Berendsen method is applied to equilibrate the temperature and then the Nose-Hoover thermostat is used to reach the target temperatures.

The two distinct approaches that are used in this simulation are the step by step and the continuous models. In both of these models, the sample temperature changes from 193 K to 793 K with an increment of 100 K. Therefore, for each of the coatings, 14 distinct simulations are performed. In the step by step approach, after each 100 time-steps of simulation, the temperature of the indentation region is returned to its initial value. But in the continuous approach, the temperature is not under control like a real test. Indeed, the both ways proposed in this study for simulation of the nano-indentation can indicate possible effects of temperature on the results. For controlling the temperature, a semispherical zone is created in the indented region as shown in Fig. 2. The temperature is recorded for each of the four thin films.

3. Results and Discussion

3.1. Deformation Mechanism

A snapshot of the cutaway view of the nano-indentation process during the simulation is shown in Fig. 3. The dislocation nucleation of a monocrystal FCC on the (1 1 1) sliding plane can be seen in Fig. 3 as depicted by black lines.

There are small dislocation regions of atoms under the indentation tip. The edge of the region is along the (1 1 1) sliding plane.

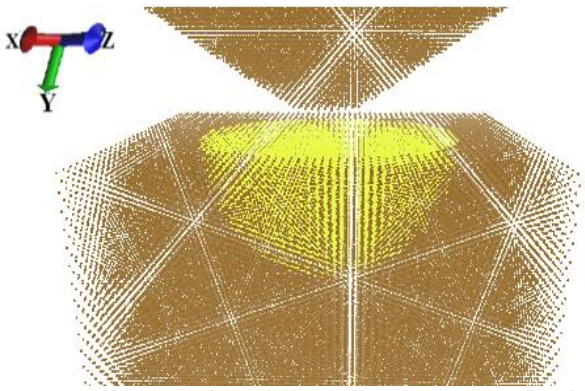

Figure 2. The semi-spherical zone (yellow atoms) created in the indentation region for controlling the temperature

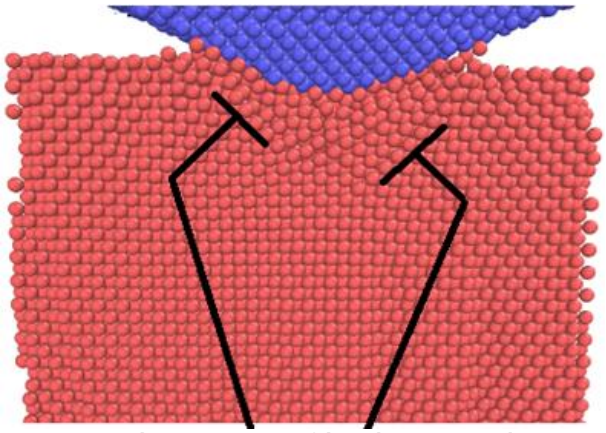

Figure 3. The cutaway view of the indentation simulation

During the indentation, when the strain energies stored in the deformed lattices exceed a certain level, atoms are rearranged successively onto the lower lattice to relax the lattice strain, and consequently a lot of dislocations are generated. The other reason for the fluctuations of the forces during the simulation is the existence of the complicated dislocation movements in the work piece during the nano-indentation process.

3.2. Elasticity Modulus

For extracting the mechanical properties of thin films, the continuous load-displacement data obtained from a complete cycle of loading and unloading during the nano-indentation test is used. The effective elasticity modulus can be calculated using the Sneddon relationship [8].

$$\frac{1}{E_{eff}}=\frac{1-\nu^2}{E}+\frac{1-\nu_i^2}{E_i} \tag{2}$$

where E and ν are the elasticity modulus and Poisson's ratio of samples, E_i and ν_i are elasticity modulus and Poisson's ratio of the indenter tip and E_{eff} is the effective elasticity modulus obtained from the nano-indentation test that can be calculated using the following equation [28]:

$$E_{eff}=\frac{\sqrt{\pi}}{2}\frac{S}{\sqrt{A_c}} \tag{3}$$

A_c is the area of the indented hole and S is the stiffness of the film which is the main parameter obtained from the load-displacement curve. This value is the slope of the unloading part of the load-displacement curve and is expressed as what follows [28]:

$$S=\left|\frac{dF}{dh}\right|_{F=F_{max}} \tag{4}$$

F_{max} is the maximum force during the nano-indentation test. For calculating the area of the indented hole in the thin film, two parameters should be considered: the indentation depth after the unloading and the geometry of the indenter tip. The proposed formula to obtain this area for a conical indenter tip can be expressed as the following:

$$A_c=\pi r\sqrt{r^2+h^2} \tag{5}$$

where r and h are the radius and height of the indented area.

The load-displacement curves obtained from the MD simulation of nano-indentation test are shown in Fig. 4. As it is shown in Fig. 4, the maximum force of indentation decreases by increasing the temperature due to the reduction in the resistance of the layers against the indenter penetration. Rising the temperature, the vibration of atoms and the nucleation of voids increase which can be considered as the reason for increasing the fluctuation in the load-displacement curves.

The elastic recovery of the indentation region also becomes less as the temperature rises, which indicates the increasing of the plastic deformation in the indented zone. The loading parts of the curves are quite fluctuating because the interactions between the indenter and material are based on the discrete atoms. But the unloading parts of the curves are relatively smooth because attractive forces approach zero in the presence of large interatomic distances.

The indentation process involves significant plastic deformation and therefore, the surface of the specimen around the indenter is typically drawn inwards (sinking-in) or outwards (piling-up). These phenomena are considered as the errors associated with this procedure and can affect the validity of the results [29]. The plastic deformation in the indented region is the main reason for the piling-up phenomenon which is observed in this study. As the temperature rises around the indenter (due to the friction between the indenter and the film surface) and also due to the interactions among the atoms, the possibility of the plastic deformation increases. The nano-indentation test is a continuous procedure which leads to an incontrollable change of temperature around the indenter that intensifies these errors. The values of elasticity modulus calculated from Eq. (2) are shown in Tables 1 and 2. The results show the differences between the temperature change in the films (which are due to the discrepancy of the interactions among the indenter atoms and the layer atoms) and also the differences between the cohesive energy among the atoms of each thin film.

In the step by step approach, the temperature of the indented region is turned to its initial value every 100 time steps. Measuring and comparing the size of the material that piled up around the indenter, the results show the differences of this value among the two applied ways which demonstrate the usefulness of the step by step approach. The piling-up amount is diminished up to 42% with respect to the values obtained in the continuous way.

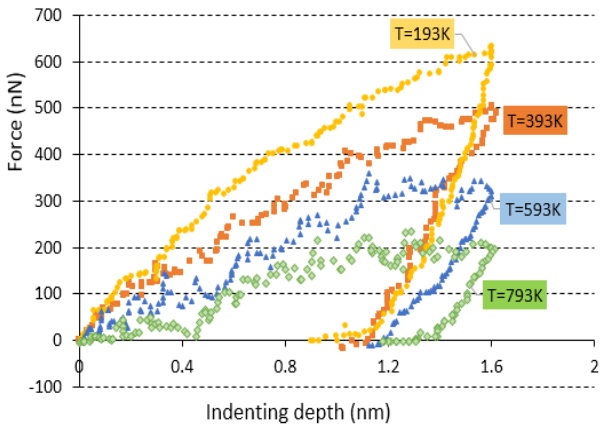

Figure 4. The load-displacement curves obtained from the MD simulation

Table 1. The elasticity moduli of the coatings obtained from MD simulation using the continuous approach (GPa)

Temperature (K)	Coatings			
	Cu	Al	Ti	Ag
193	148	109	205	119
293	128	95	174	106
393	106	79	161	91
493	85	64	150	78
593	63	47	138	68
693	45	33	127	54
793	30	19	117	51

Table 2. The elasticity moduli of the coatings obtained from MD simulation using the step by step approach (GPa)

Temperature (K)	Coatings			
	Cu	Al	Ti	Ag
193	153	122	218	128
293	135	110	185	114
393	112	91	174	102
493	90	73	160	82
593	79	53	146	68
693	61	38	137	48
793	54	22	123	32

Comparing the calculated values reported in Tables 1 and 2, it is obvious that the elasticity modulus decreases by increasing the temperature. This reduction is due to the increase in the ratio of the plastic deformation in the indented region against the elastic deformation. It should be noted that by increasing the temperature, the amount of the defects and voids in the structure of the films increases which leads to the extension of the amorphous section in the crystalline structure of the films. The fact that the values obtained from the step by step approach are higher than the ones obtained from the continuous way can be seen from the results. As the temperature of the indentation region is not controlled in the continuous approach, this rising leads to the elevations in the velocities of atoms and also the interactions among the atoms that cause the decline of the binding between the atoms and the reduction in the elasticity modulus.

To compare the results with other results of other studies, a theoretical model available in [30] is considered:

$$\frac{E(T)}{E_0}=\frac{1-\frac{C_V T}{U_0}}{(1+\alpha T)^3} \quad (6)$$

Where E_0 and U_0 are the elastic modulus and the cohesive energy at 0 K, respectively. Equation (6) indicates that the temperature-dependent elastic modulus $E(T)$, can be obtained by the cohesive energy at 0 K, the specific heat C_v, and the thermal expansion coefficient α [30]. Figs. 5-6 show the temperature-dependent elastic modulus of Cu and Ti thin films. Al and Ag trends are similar to those of Cu and Ti.

As it can be seen in Figs. 5-6, at low temperatures the difference between the simulation results and the theoretical model is negligible (the difference is less than 5%). But by increasing the temperature, the discrepancy becomes greater (up to 34%). This difference is due to the existence of the defects and voids in the simulation models.

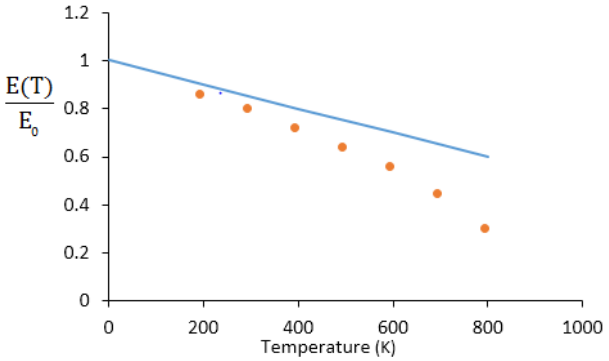

Figure 5. The temperature-dependent elastic modulus of Cu thin film. The lines are predictions based on Eq. (6). The points are the results of MD simulations.

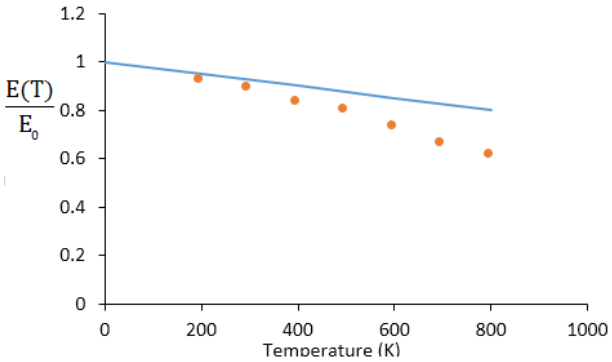

Figure 6. The temperature-dependent elastic modulus of Ti thin film. The lines are predictions based on Eq. (6). The points are the results of MD simulations.

As temperature increases, the amount of the defects and voids in the structure of the films becomes larger, and hence the elastic modulus decreases.

3.3. Hardness

For measuring the material hardness H, a simple equation is used which is determined by dividing the maximum load of nano-indentation P_{max} to the projected contact area A_c [3].

$$H=\frac{P_{max}}{A_c} \quad (7)$$

The simulation results were substituted into Eq. (7) and for both of the applied approaches the hardness values of thin films were obtained. Tables 3 and 4 show the hardness values determined for Cu, Al, Ti and Ag coatings at different temperatures. Both of the parameters used to calculate material hardness was affected by temperature.

By increasing the temperature, the maximum load (P_{max}) decreased and the projected contact area increased. The reasons for these trends are the same as the ones described earlier for the elasticity modulus.

By comparing the values given in Tables 3 and 4, it is seen that the hardness values obtained from the step by step approach are more than the corresponding values from the continuous approach. This discrepancy varies from 2% up to 19% with highest values related to the low temperatures. In general, as the temperature rises, the discrepancy becomes smaller.

Table 3. Hardness values of the coatings obtained from MD simulation using the continuous approach (GPa)

Temperature (K)	Coatings			
	Cu	Al	Ti	Ag
193	5	4.9	9.5	3.9
293	4.8	4.7	8.8	3.6
393	4.5	4.3	8.3	3.2
493	4.1	4	8.1	2.9
593	3.5	3.3	7.7	2.5
693	3.2	3	7.4	2.3
793	2.6	2.5	7	2

Table 4. The hardness values of the coatings obtained from MD simulation using the step by step approach (GPa)

Temperature (K)	Coatings			
	Cu	Al	Ti	Ag
193	5.9	5.8	10.5	4.7
293	5.3	5.3	9.6	4.4
393	5	4.9	8.9	3.9
493	4.5	4.5	8.5	3.6
593	3.8	3.6	8.2	3.2
693	3.3	3.2	7.8	2.6
793	2.7	2.5	7.4	2.2

Due to the lacking data from the experimental studies in which the same conditions are applied as the present simulations, the results of the current simulation for Cu are compared with the Young's modulus found experimentally by Lebedev et al. [31] and material hardness reported by Hung et al. [32]. Lebedev et al. obtained the Young's modulus of copper as approximately 116-126 GPa (when the temperature changed between 20 and 300°C), while the present MD simulations found it as 54-153 GPa (when the temperature changed between 193 and 793 K). The difference is less than 10% at low temperatures while at higher temperatures, it increases up to 50%. Hung et al. have reported the hardness of copper as approximately 0.9-4.4 GPa (when the temperature changed between -190 and 60°C), while the present MD simulations determined it as 2.6-5.0 GPa (when the temperature changed between 193 and 793 K). The values of hardness obtained in our simulation are significantly larger than those reported by Hung et al. [32]. This relatively large discrepancy can be a result of the scale difference between the experiment and simulation, i.e. micro-scale and nano-scale. In fact, the effects of the defect on the deformation mechanisms of material are different at different scales.

4. Conclusion

In this study, the nano-indentation process was simulated using molecular dynamic method to evaluate the temperature effects on the mechanical properties of thin film coatings made of Cu, Al, Ti and Ag. It is demonstrated that the elasticity modulus and hardness decrease when the temperature increases. The effect of temperature changes was more dominant on the measured hardness than on the elasticity modulus. The main reasons for these declines are the increase in the defects and voids in the crystalline structure of the thin films and the increase in the plastic deformation with respect to the elastic deformation. This means that elastic recovery reduces as the temperature increases.

The effect of local temperature elevation in the indentation region due to the interactions between the indenter and the layer atoms was also studied in this study. This local temperature increase, that is avoidable in a real test, enhances the plastic deformation in the indentation zone which leads to the intensification of the piling-up phenomenon. For decreasing such effects, the step by step approach was proposed as a useful simulation way.

Nomenclature

FCC	Face centered cubic
HCP	Hexagonal close packed
p	Pressure
H	Hardness
A_c	Contact area
E	Elasticity modulus

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