Modeling and study of a rough Nickel sample

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ABSTRACT: This work presents the study of the creation of dislocation and defects by the compression of a rough sample of nickel. The random surface has been created using a home-made script and all the simulations were made using LAMMPS. Atomsk and Ovito software were used for creation of the sample and visualization. This work shows a reduction in the Young modulus and yield strengths with a reduction of the degree of roughness.

I. Introduction

The use of molecular dynamics (MD) simulation to study the structural properties of molecular system has become an important tool to predict the and understand the behavior of such systems. In our work, the dislocation occurred after the compression of a sample has been investigated. The presence of dislocations has important influences on several properties of the material. This study provides the results of the simulation of the compression of a rough sample of nickel. Recently studies indicate that the shape of the surface could change the mechanical properties of a nanoparticle [1]. A comparison of the mechanical properties of a rough and smooth sample has thus been investigated. The rough surface of the sample was simulated using a home-made script. All the simulation was done using LAMMPS and the visualization of the compression was done using Ovito. The dislocation of a smooth and a rough sample was compared, as the influence of the roughness of the sample.

II. Method

A cube of nickel nanoparticles was created using Atomsk software [2]. The procedure includes the specification of the kind of particle, the lattice parameter, the lattice type (fcc) and the repetition of the previous structure in the three dimensions. Once created, the nanoparticles, the six faces of the sample are perfectly flat. One-face-rough nanoparticle was created by intercepting the uppermost atom layers of the perfect flat sample with the random surface created with a point density matching the atom position.

II.1 Random surface generation

Mathematical generation of random surface (RS) has been widely discussed in previous works. Generally, the RS has been classified in anisotropic or isotropic (considering the changes in properties along the surface). Also taking considering the height distribution the RS can be classified in Gaussian or not Gaussian. In this work we will be generating Homogeneous isotropic Gaussian RS. Among the principal methods used for random surface generation we can mention the linear transformation, 2-D filters [3] and time series model [4]. Here we will be using a simple method where a periodic function is randomly modified in amplitude and phase.

$$\mathbf{z} = \mathbf{C1} * \sum_{\mathbf{n}=-\mathbf{N}}^{\mathbf{N}} \sum_{\mathbf{m}=-\mathbf{M}}^{\mathbf{M}} \left(\boldsymbol{m}^2 + \boldsymbol{n}^2\right)^{-b/2} * \mathbf{G}(\mathbf{n},\mathbf{m}) * \mathbf{cos}\left(\mathbf{2\pi}(\mathbf{mx} + \mathbf{ny}) + \mathbf{U}(\mathbf{n},\mathbf{m})\right) \quad (\mathbf{1})$$

The height distribution is given by equation 1. G(n, m) and U(n, m) are the matrix array of Gaussian and Uniform

distributed random numbers respectively in the interval [0, 1] and $[-\pi/2, \pi/2]$. **C1** is a normalization factor. **X** and **Y** are the Cartesian locations where the height will be determined. The parameter b can be seen as a spectral exponent and it will parameterize how fast the high frequencies are attenuated. If the final height for random surface follows a Gaussian distribution the standard deviation (σ) represents the main parameter for such characterization. If the mean value of height (l) is zero, the standard deviation coincides with the RMS and can be also used to characterize the degree of roughness.

$$\sigma = \sqrt{\frac{1}{NM}\sum_{i=1}^{NM}(z_i - l)^2} \qquad (2)$$

II.2 Molecular dynamics

In molecular dynamics (MD) the position and velocities of particles are determined by solving numerically the equation of motion. The potentials of interaction between particles should be expressed as well as the thermodynamic ensemble constraining the system. The external perturbation (if any) must be defined and the initial and boundary conditions. With that, a numerical algorithm will integrate the second Newton law for all particles present in the sample and the dynamics parameters will be determined every time step defined by the simulation setup. The resulting thermodynamics parameters needed will be obtained in function of the ensemble defined for calculations.

II.3 Modeling conditions

The compression of the nanoparticles was done using LAMMPS software [5]. Before compression, the nanoparticle was minimized. The system was heated to 300K and then equilibrated to finally be compressed in Z direction. For the interaction potential between the atoms was chosen the Embedded Atom Method (EAM) due Finnis and Sinclair [6].

A minimization is the first step required in almost all studies using MD. It sets the system at the minimum or very near to the minimum energy configuration. With this, the experiment will be more similar to real conditions and the stability of the numerical integrator used is guaranteed. The system was minimized using conjugate-gradient method with stopping tolerance for energy (etol) and force (ftol) settled as 1 and 10^7 respectively. The maximum iteration (maxiter) was chosen as 10000 and the maximum number of evaluation for force and energy (maxeval) as 100000. Another step is to run a relaxation. With this the box size and shape are allowed to vary. After the minimization the system was settled at room temperature (300K). The introduction of velocities in the atoms by setting temperatures may change the stability of the sample and make the temperature drop down. The system should be equilibrated to guarantee the Kinetic and Potential energy to distribute evenly through the sample. It was done using NPT ensemble (constant pressure temperature and number of particles), which is the condition similar to most experimental setup and is the widely used during equilibration in MD. The sample was equilibrated at 300 K during 20 ps using the Nosé–Hoover thermostat [7].

The compression of the nanoparticles was performed after the previous steps. The rough surface of the sample was located perpendicular to Z axis, so the uniaxial compression was performed in that direction. The strain rate was chosen as 0.01 ps^{-1} and the process run for 20 ps at constant pressure, temperature and number of particles. The constrain to pressure during this step was performed only to the faces in X and Y directions. The deformation process in Z direction do not allow to constrain also the pressure.

III. Results and discussion

Using Atomsk [7] software, a nickel cubic sample (fcc) was created with lattice parameter of 0.352 nm. After a minimization process it was found a lattice parameter of 0.3518 nm as the best option for a minimum in energy. A cubic sample of 8.7952 nm lateral size containing 62500 atoms was created using the new lattice parameter for be used in the compression model.

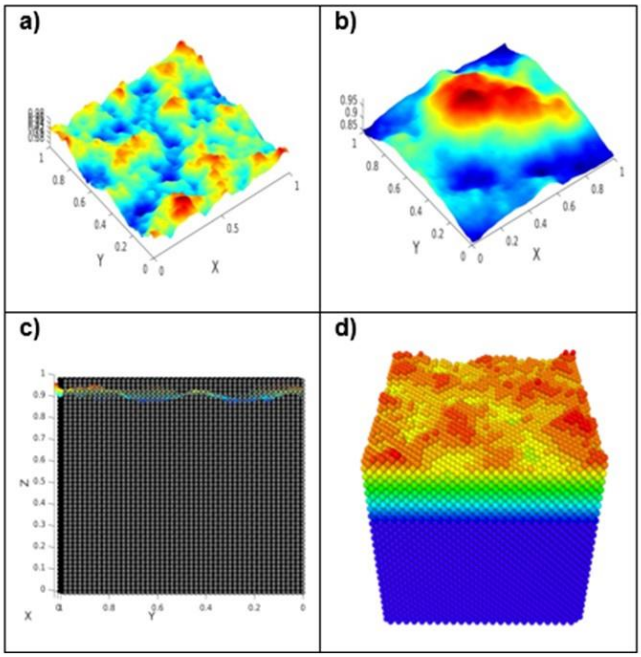

Figure 1: (a) Rough surface with b=1.6. (b) Rough surface with b=2. (c) Interception of a cubic nanoparticle made of nickel atoms with the rough surface generated with b=2. (d) Nickel nanoparticle after remove the atoms over the surface.

Random surfaces with different roughness degree were created using equation 1. Two roughness levels were evaluated for spectral exponent b taking values of 1.6 and 2 (figure 1 a) and b) respectively). The parameters N=M were assumed as 30 and C1=0.01. RMS values of 0.0185 and 0.0294 were obtained for b equal to 1.6 and 2 respectively. X and Y were chosen to be in the interval [0,1] with step size matching the number of atoms present in X or Y direction in the sample. It was done using cfg format in Atomsk for the generation of the sample.

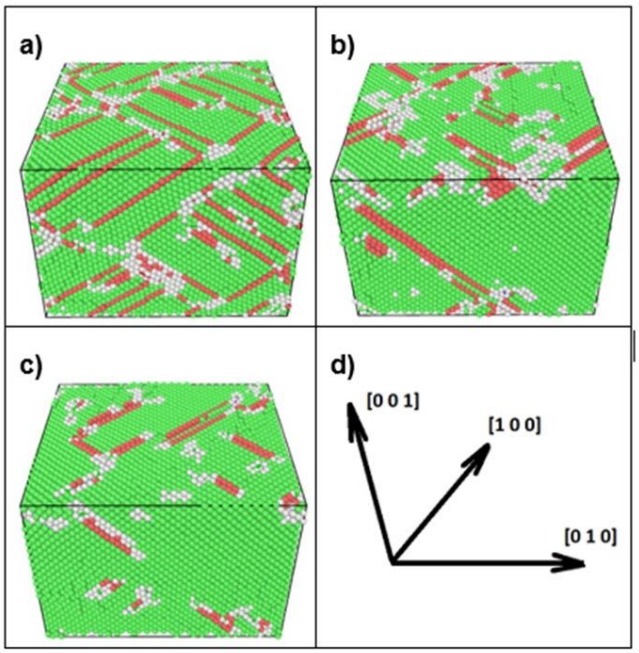

Figure 2: Dislocation analysis with Ovito for a (a) perfect flat nickel nanoparticle, (b) rough surface with b=1.6, (c) rough surface with b=2. (d) Crystallographic direction schematically represented.

Table 1. Yield strengths and Young modulus for three samples.

Sample	Yield strengths (GPa)	Young modulus (GPa)
planar	8.247	132.2
b=1.6	4.504	106.1
b=2	3.162	42.85

Next, the rough samples were created by intercepting the maximum height of the rough surfaces with the uppermost layer of atoms (figure 1 c)). After, the atoms over the surface were removed. Finally, the sample was converted to LAMMPS format (figure 1 d)). After the process of remove the atoms the two samples contained 58048 and 56871 atoms for the cases of b=1.6 and b=2 respectively.

Before the compression; the samples were equilibrated at 300 K during 20 ps following the procedure explained in method section. The positions of some atoms in the top part were slightly changed as a consequence. Then a compression process with strain rate of 10^{10} s^{-1} was performed in Z axis for the three nickel nanoparticles.

The calculation process was performed using LAMMPS running over Ubuntu 16.04 in HP laptop computer system. The system poses 4 Giga DRR3 RAM memory and CORE I5 at 2.4 GHz microprocessor. In these conditions every simulation took around of 2 hours 30 min.

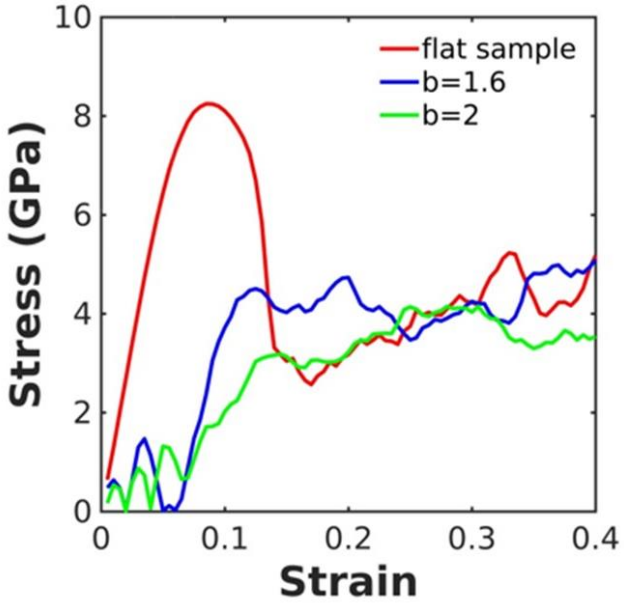

Figure 3: Strain-Stress curve obtained from the compression of the different nanoparticles. Sample with flat surface is represented in red. The samples made with interception of rough surfaces made with b=1.6 and b=2 in blue and green respectively.

Figure 2 shows the dislocation analysis made with Ovito for the three samples at strain value of 0.2. The flat sample (figure 2 a)) shows more presence of hexagonal closed-packed atoms (red atoms) and more dislocation process. However, the fcc crystal type still the majority for all three samples. Figure 2 d) represent the schematically representation used in this study where X=[100], Y=[010] and Z=[001].

During the compression, the two rough samples show changes in the crystallographic structure at early stages. Most of these changes were observed very near to the surface where the roughness was previously created. It may be explained by the re-accommodation of the atoms

located at the top surface when the compression is initiated.

Strain-stress graph (figure 3) shows the clear evidence in the mechanical properties between a flat and a rough surface nanoparticle. The rough nanoparticles show instability at the beginning of the curve followed by a more stable liner regimen. For the case when the roughness is high is simple to estimate a value for Young modulus and yield strengths (table 1) in the linear part immediately after the re-accommodation process. In the same way, the mechanical parameter was calculated for the b=2 rough nanoparticle. In the last case the linear part after the three first maximum was taken into account for Young modulus estimation and the Yield strength.

Conclusion and outlook

This study shows the variation in mechanical properties of a Nanoparticle with rough surfaces when it is compared with a flat one. The results indicate a reduction of the yield strength and Young modulus with a reduction of the degree or roughness. As a continuation of this work; further studies at different compression rate and different sizes must be done.

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