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DEFORMATION OF A SINGLE ASPERITY BY A RIGID FLAT PLATE: A MOLECULAR DYNAMICS STUDY[1]

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Abstract
Contact mechanics is a subject with a wide spectrum of applications and is central to the study of tribology. In the present work the problem of a single metallic asperity brought into contact with a flat rigid plane was studied using molecular dynamics (MD). The molecular dynamics calculations were performed using the LAMMPS code with interatomic potentials described by the embedded atom method (EAM). The asperity was deformed by the rigid plane at a constant speed of 1m/s. The normal force acting on the rigid plane, energy, temperature and contact radius were monitored to study the atomic mechanisms involved in the deformation process. The results indicated a significant hysteretic behavior for the formation and fracture of the junction.
Key words: Tribology; Simulation; Molecular dynamics.

DEFORMAÇÃO DE ASPEREZA POR UM PLANO RÍGIDO: UM ESTUDO POR DE DINÂMICA MOLECULAR

Resumo
A mecânica do contato é um tópico com um espectro amplo de aplicaçoes e é um tema central na tribologia. O presente trabalho trata da deformação de uma aspereza metálica por um plano rígido por meio de simulações de dinâmica molecular (MD). As simulações de dinâmica molecular foram realizadas por meio do código LAMMPS e as interações atômicas de acordo com o "embedded atom method" (EAM). A aspereza foi deformada pelo plano rígido a uma taxa de 1 m/s. A força normal que age sobre o plano rígido, energia, temperatura e raio de contato foram monitoradas durante a simulação com o objetivo de estudar os mecanismos atômicos envolvidos no processo de deformação. Os resultados indicaram que o processo de formação e fratura da junção apresenta comportamento histerético pronunciado.
Palavras-chave: Tribologia; Simulação; Dinâmica molecular.

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1 INTRODUCTION

When two solid bodies are brought into contact the interaction between them does not occur at the whole of their macroscopic contact area, but only in places where their asperities touch each other. Upon contact, numerous junctions are formed and interfacial effects like wear, adhesion and friction depend on its behavior. The classical approach to treat contact problems is the use of continuum theories such as Hertz theory[1] which can treat analytically single asperity contact problems. This model assumes that the asperity strains are elastic and does not take into account the effects of adhesion. The effects of adhesion on contact problems can be treated with the Johnson, Kendall and Roberts (JKR) model[2] which assumes that adhesion forces act between the surfaces only within the contact region (short range interactions). In this model the adhesion component is introduced via a term which represents the work of adhesion between the solids. The Derjaguim, Muller and Toporov (DMT)[3] is another model which deals explicitly with adhesion. In this case, however, adhesion forces are considered to act beyond the contact area (infinite range interactions).

Since asperities sizes can range from a few micrometers down to a few nanometers the approximation of the structures of the bulk and material surface by continuous functions at this scale becomes unreliable at best. Therefore the use of continuum based models at these scales cannot be justified. A complete understanding of interfacial phenomena can only be achieved by means of simulations and experiment at the same length scale. To this end, molecular dynamics (MD) simulations can be successfully used in the study of nanometer-sized contacts since it takes into account the discreteness of atomic structure and it provides a way to observe the physical phenomena taking place at this small scale.[4]

There are several works in the literature that treat the contact of a single asperity at the nanometer scale. For instance, Cha, Srolovitz, and Vanderlick[5] studied the constant temperature deformation of a single gold asperity by a rigid plane through MD simulations. Their results showed that during loading partial dislocations are created and emitted and that there is an extensive elastic deformation during unloading. Song and Srolovitz[6] used the same geometry used in Cha, Srolovitz, and Vanderlick[5] and showed that adhesion has little effect during loading of the asperity, when the junction is formed, but it influences the separation (unloading) process. Fortini et al.[7] studied the contact between Au and Ru asperities at 300 and 600 K and showed that the fracture of these contacts could be ductile or brittle depending on the temperature. In all these works the temperature was held constant during the simulations.

During the plastic deformation of a metal, heat is generated and conducted away from the source point. If the deformation process is carried at high rates it can be considered essentially as an adiabatic process since there is not enough time for the conduction of heat. The adiabatic deformation seems to be, in the context of MD simulations, a better assumption than the isothermal one since timescales available to this technique are of the order of nanoseconds.

The aim of this paper is to study the contact of a single Ni asperity deformed by a rigid plate using MD simulations. In the present work no temperature control was performed in order to include the effect of this variable in the analysis of the problem.

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2 SIMULATION PROCEDURE

All MD simulations in this work were performed using the LAMMPS code[8] with atomic interactions described by the Embedded-Atom Method (EAM).[9] In the present work the EAM potential for nickel (Ni), with a lattice constant of 0.352 nm and fcc structure, developed by Foiles et al will be used.[10]
The system geometry was constructed with a rigid plate and a half-sphere placed on the top of a deformable slab. The deformable slab has dimensions of 7.7 x 7.7 x 2.2 nm and the half-sphere has a radius of approximately 2.0 nm. The total number of atoms in the simulation is 20297. The atoms belonging to the bottom layer of the deformable slab were held immobile during all simulations.
Since the system geometry was constructed from a perfect fcc lattice at 0 K and the simulations of the asperity deformation were made at finite temperatures, an equilibration treatment was performed so the system could reach the equilibrium configuration at the start temperature of the asperity deformation (300 K). In the equilibration cycle the system was kept at constant temperatures of 1350, 1000, 700 and 300 K during 0.25 ns for each temperature. Test runs showed that for this duration the system energy, after a initial transient, was conserved and did not show any drift (i.e. a slow energy variation with time). During the equilibration cycle the number of atoms, volume and energy were kept constant (NVE ensemble) using the velocity-Verlet algorithm with a time step of 0.001 ps.
The atomic configuration after the equilibration cycle is shown in Figure 1. The resulting geometry shows facetting of the top and lateral planes of the asperity due to differences in surface energy with crystallographic orientations.

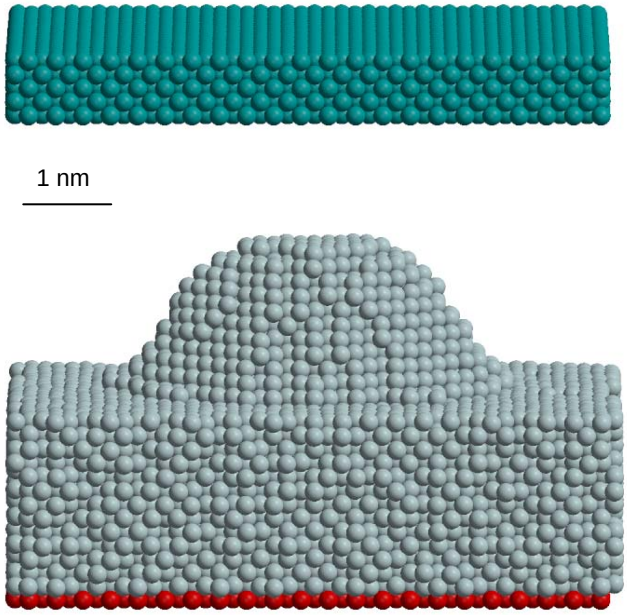

Figure 1: System configuration obtained after the equilibration cycle.

The asperity shown in Figure 1 was deformed by displacing the rigid plane towards the asperity by an increment of 0.0001 nm every 0.1 ps (100 timesteps) providing a loading/unloading rate of 1 m/s. The total rigid plane displacement during the loading cycle was 0.6 nm at which time its movement was reversed and the unloading cycle began. During the unloading cycle the rigid plane was displaced at the same speed of the loading stage until complete fracture of the junction formed. The force acting

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on the rigid plane was monitored during all simulations and was calculated as a sum of the vertical components of the forces acting on every atom of this body. No temperature control was performed.
The contact radius at the loading stage was calculated using the coordinates of the atoms generated by the simulation according to a procedure proposed in Vergeles et al.[11] First the atom with the highest y coordinate (not considering the atoms of the rigid plane) was identified and them all atoms with coordinates between y and y - 0.5*s* were selected. *s* is an empirical parameter of approximately 65% of the Ni lattice spacing suggested in Vergeles et al.[11] The contact radius was calculated using this group of atoms through the formula:

$$\frac{a^2}{2} = \frac{\sum\left[\left(x_i - x_{cm}\right)^2 + \left(z_i - z_{cm}\right)^2\right]}{N}$$

Where *a* is the contact radius, *N* is the number of selected atoms, x_i and z_i are its *x* and *z* coordinates and x_{cm} and z_{cm} are center of mass coordinates of this group of atoms.

3 RESULTS AND DISCUSSION

3.1 Loading Stage

Figure 2 shows how the normal force acting on the rigid plane, contact radius and energy of the system vary with the separation of rigid plane - asperity during the loading stage (the dotted vertical lines are a visual aid in the interpretation of the results). It can be seen from this figure that the normal force varies in a nonlinear manner with the separation distance. Initially the force is zero for distances greater than 0.45 nm and the total energy remains constant up to this point. Further approach between the two bodies causes an abrupt drop of the normal force to its minimum value at approximately 0.4 nm. From this point on a series of events take place where the force increases to local maximum and then suddenly drops to a local minimum. It is interesting to note that these drops in the force curve (Figure 2c) can be associated with inflexions of the energy curve (Figure 2a).
The initial force drop is towards negative values, and therefore of an attractive nature, and occurs when the separation between the asperity and the plane reaches a critical value of approximately 0.4 nm. At this critical distance, which is very close to the lattice spacing of Ni (0.352 nm), the surface atoms at the top of the asperity are attracted towards the rigid plane causing deformation of the asperity at zero load. The sudden increase of the contact radius to a value of approximately 0.7 nm indicates that at this point contact is established between the asperity and the rigid plane (see Figure 3). This result is consistent with previous MD simulations results found in the literature,[9,10,12,13] and is known as the jump-to-contact phenomenon (JC) or adhesion avalanche.[14]
The JC is related to a competition of attractive forces which act across the asperity/rigid plane gap and the binding effect of the atoms in the sub-surface layers. The adhesive force acting between the two bodies is capable of inducing strains on the asperity even when no external load is applied. However this deformation involves the first three or four atomic layers of the asperity and the surface atoms moved a distance of 0.1 nm in a time frame of approximately 2 ps. Observation of the asperity surface (Figure 3) showed that the deformation did not occur in a elastic

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manner since there is some change of the surface asperity, as already pointed out in Cha, Srolovitz, and Vanderlick.[5]

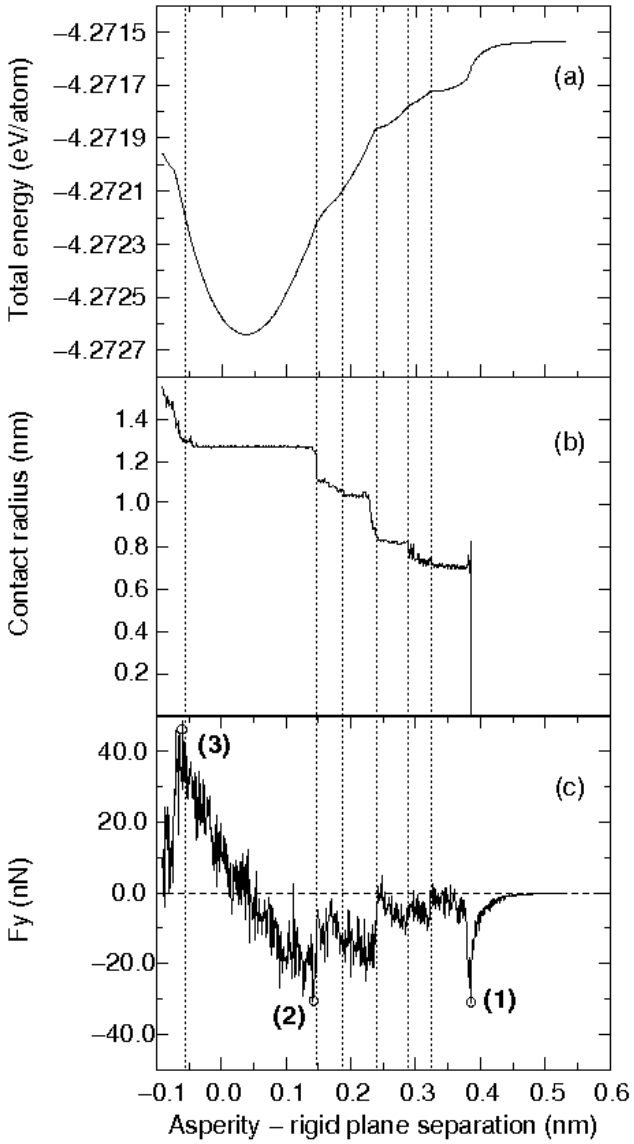

Figure 2: Normal force, contact radius and total energy per atom versus asperity/rigid plane separation distance obtained during the loading stage.

Upon further approach of the rigid plane (beyond point labeled **1** in Figure 2c) the normal force, as already noted before, increases and then drops to a local minimum. Each of these events is associated with a change of inflexion of the energy curve, while the contact radius remains fairly constant.

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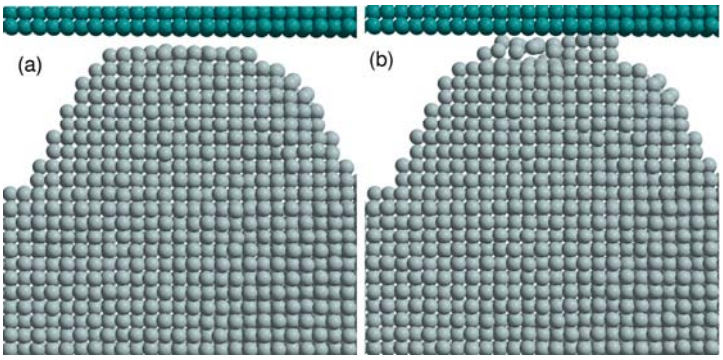

Figure 3: Jump to contact phenomenon: (a): snapshot of the system just before the rigid plane reaches the critical for the occurrence of the JC (b): snapshot of the system where the deformation of the asperity due to adhesive forces can be seen.

The contact radius increases in a stepwise fashion as the force suddenly drops. With continuing deformation, beyond point **(2)** in Figure 2c, the normal force increases almost linearly with deformation, the contact area remains constant and the energy varies almost parabolically, decreasing at first and then increasing. Similar results can be found in the literature. Cha, Srolovitz, and Vanderlick[5] explained this behavior by means of the generation and movement of structural deffects (dislocations and stacking faults) generated by the deformation. Fortini et al.[7] also explained the observed force drops in the force versus distance curve by means of generation and movement of deffects. Sorensen, Brandbyge and Jacobsen,[15] analyzing the tension of an atomic contact, attributed this kind of behavior to the fact that the deformation occur by a two stage process: a rearrangement of the atomic structure followed by a stage of elastic deformation, where the atomic structure remains virtually unaltered. Detailed analysis of the atomic structure performed by the authors of the works cited above showed the creation and movement of deffects during the deformation. The generation and movement of deffects is a reasonable explanation for the behavior observed in the present work. In a thermodynamic sense, work is performed on the asperity by the rigid plane resulting in an overall increase of the system energy if it were not by the deffects created which cause the system to relax and decrease its energy.

During the loading stage the temperature of the system remains constant at first and then increases linearly once contact is established between the rigid and asperity as shown in Figure 4. At the final portion of the loading stage there is a sharp increase of the temperature of approximately 10 K concurrent with a relatively large force drop (point **3** in Figure 2c). It seems that the temperature of the system is not connected to the smaller force drops that occur before this point. It is worth noting that the energy at this portion of the loading cycle varies almost parabolically decreasing at first reaching and after reaching a minimum starts to increase (points **2** and **3** of Figure 2c). The relationship between the increasing energy and temperature at this stage is difficult to establish. It could be that the system, at this region, has exhausted its ability to accommodate the deformation through the creation of deffects. The atoms then assume positions of higher energy without any noticeable restructuring thus causing the energy of the system to increase as shown in Figure 2. Since temperature and energy are intimately connected this could explain the elevation of the measured temperature rise of the system. However it does not explain why there is an increase in temperature while the energy decreases.

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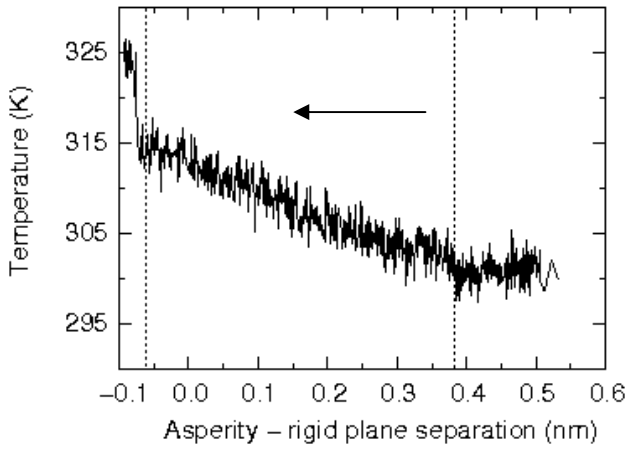

Figure 4: Temperature of the system during the loading stage.

3.2 Unloading Stage

The variation of the normal force versus separation distance at the unloading stage is presented in Figure 5. Initially the force varies linearly with increasing separation and once it reaches a minimum slowly approaching zero at large separation. During this stage sharp force drops can also be observed as in the loading stage.

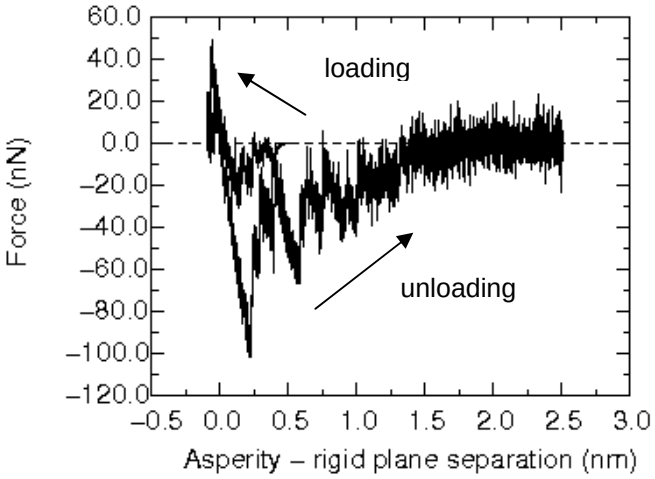

Figure 5: Normal force versus separation for loading and unloading cycle.

The asperity and plane separate at a much larger separation distances than at which the contact occurred (approximately 0.4 nm). Figure 6 presents a snapshot of the system just before the fracture of the junction. It can be seem from this figure that the separation of the solids does not occur at the asperity -rigid plane interface but a t the bulk of the asperity. Also there is an extensive material transfer due to adhesion from the asperity to the rigid plane. A strong adhesion between the surfaces of the asperity and the rigid plane is to be expected since the two solids are in perfect registry and the contact is established along the (010) crystallographic plane. The amount of material transferred depends on the interfacial energy of the solids.[6]

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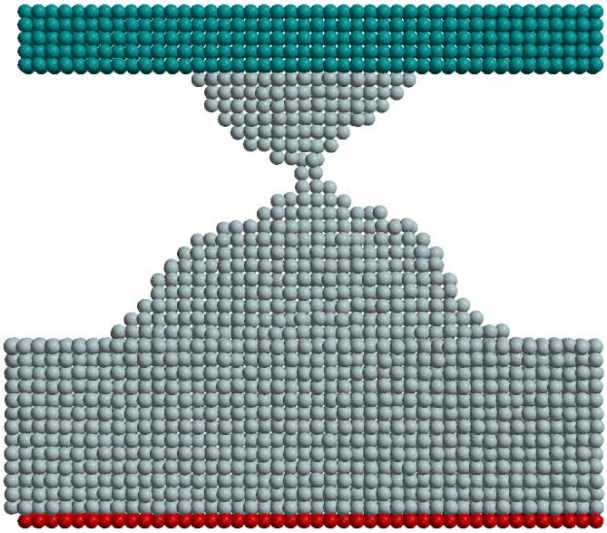

Figure 6: Snapshot of the asperity and rigid plane just before fracture of the contact.

The system temperature during the unloading stage varied in a stepwise manner as shown in Figure 7.

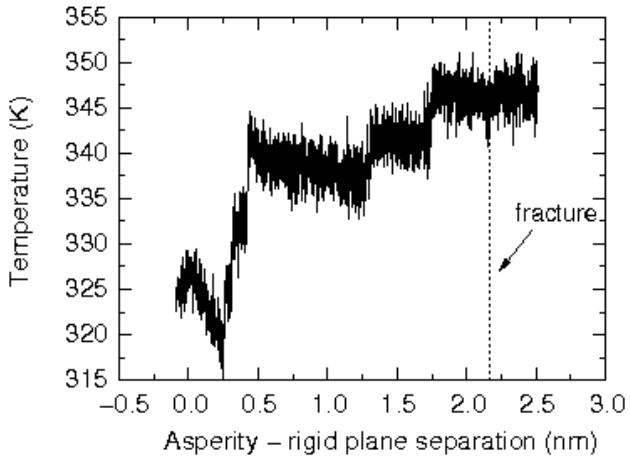

Figure 7: Temperature variation during the unloading stage.

At first there is a decrease in temperature with increasing separation of the two bodies followed by a sharp increase in temperature of approximately 25 K. With continuing separation the temperature shows at first a slight tendency to decrease followed by two plateaus of constant temperature separated by sharp increases of approximately 5 K. The energy variation of the unloading cycle shown in Figure 8 does not show any remarkable features that could be linked to the temperature variation shown in Figure 7. The hysteretic behavior of the system is clear from Figure 8 where the energy variation of the loading cycle is included for comparison. The energy expended to fracture the junction formed is much higher than the energy expended during its formation. The trend show by the energy during the unloading is of increase as the rigid plane recedes. At the final stages of the unloading there is an inflexion of the energy curve (at a separation of approximately of 1.25 nm) followed by a plateau at a point before the fracture of the junction. Again, establishing a relationship between the temperature and energy variation is difficult at this moment and further studies are necessary.

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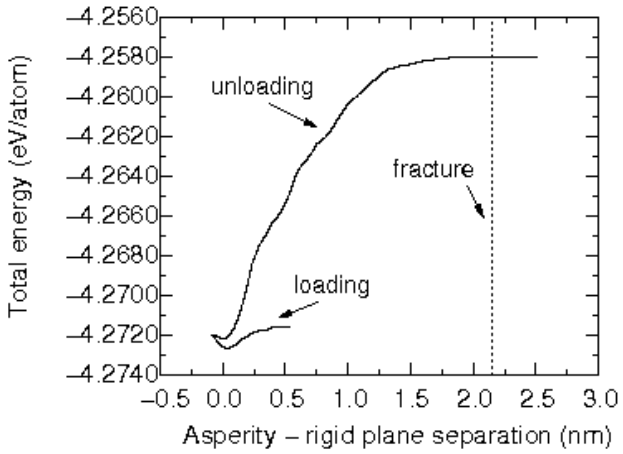

Figure 8: Energy variation during the loading and unloading of the asperity.

4 CONCLUSIONS

In this work molecular dynamics simulations of the contact between a single Ni asperity and a rigid plane were performed. The results in the present work reproduce some of the well-established results found in the literature. The adhesive forces acting between the asperity and rigid plane gap are capable of inducing strains in the system effective establishing contact even at zero load. Also the loading/unloading cycle showed a remarkable hysteretic behavior: the work necessary to fracture the junction formed during the loading stage is much higher than the work expended in its formation (adhesion hysteresis). The contact radius was measured during the loading stage and it increases in a stepwise fashion concurrently with drops in the normal force (Figures 2a and 2c) and remains constant with increasing deformation. These results are connected with the creation and movement of deffects generated during the deformation.[5,7,15]

The behavior of the temperature changes during the loading and unloading cycles were measured in order to try to verify its effect in the deformation process. During the loading stage a linear increase in the temperature was measured while in the unloading stage the temperature varied in a stepwise manner. However the relationship between energy, temperature and deformation could not be established at this moment and further studies are necessary.

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