

MOLECULAR DYNAMICS SIMULATIONS OF PLASTIC  
DEFORMATION OF METALLIC SURFACESSIMULACIJE PLASTIČNE DEFORMACIJE KOVINSKIH POVRŠIN  
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doi:10.17222/mit.2016.334

An understanding of the physical properties of a wide array of geometries is important in the quest for ever smaller and more fine-tuned devices and their parts. Surfaces play a key role in the deformation of nano-scale systems. Molecular dynamics simulations of compressive and tensile deformation were performed on nickel and copper thin films with (111), (9 9 11) and (10 10 8) surface orientations at 10 K. The (9 9 11) and (10 10 8) surfaces are vicinal to (111) and consist of a series of equidistant monoatomic steps. All the cases exhibit a yield stress asymmetry, with the yield stress being higher in compression than in tension. The near-surface region is the first to plastically deform and dislocations nucleate at the surface. The influence of the surface is most pronounced for the cases of the (10 10 8) surfaces deformed in compression, where parallel stacking faults nucleate at the steps on the surfaces in both materials, overriding the primary slip systems.

Keywords: molecular dynamics (MD), metallic surfaces, thin films, deformation

Dobro razumevanje mehanskih lastnosti široke palete geometrij je pomembno pri izboljšavah vedno manjših in zahtevnejših naprav in njihovih delov. Površine igrajo pomembno vlogo pri deformaciji sistemov na nano-skali. Z metodo molekularne dinamike smo raziskali deformacijo (111), (9 9 11) in (10 10 8) orientiranih nikljevih in bakrovih tankih filmov ob raztezanju in krčenju pri temperaturi 10 K. Površini (9 9 11) in (10 10 8) sta sosednji nominalni površini (111) in sta sestavljeni iz ekvidistantnih stopnic. Vse površine imajo asimetrično mejo plastičnosti, ki je višja pri stiskanju kot pri raztezanju. Območja tik pod površino se najprej deformirajo in dislokacije izvirajo na površinah. Vpliv površine je najbolj izrazit za primera orientacije (10 10 8) pri stiskanju, ko se oba materiala deformirata s serijo vzporednih napak zloga, ki izvirajo iz stopnic na površinah in, ki nadomestijo primarne drsne sisteme.

Ključne besede: molekularna dinamika (MD), kovinske površine, tanki filmi, deformacija

## 1 INTRODUCTION

Experiments at the nanoscale can be very time consuming and costly, in addition, they often turn out ambiguous due to lack of constraint on the thin foils examined. Such experiments also require expensive equipment and sensors, which further motivates us to use atomistic simulations to better understand deformation mechanisms at the nanoscale. Molecular dynamics (MD) simulations can serve as an effective tool for analysing dislocation nucleation mechanisms in metallic materials.<sup>1-4</sup>

Whereas the misorientation of adjacent grains determines the precise positioning of the atoms close to the boundaries, leading to diverse defect nucleation sites, the surface condition similarly influences the mechanical response of a material to external loads or deformation due to the relaxation of the topmost layers minimizing the surface energy and the adjacent free space into which the atoms can move.<sup>5-8</sup>

Vicinal surfaces, such as (10 10 8) and (9 9 11) investigated here, are produced by cutting a crystal close to a dense plane, and consist of terraces divided by equidistant monoatomic steps. When cutting or growing poly-

crystalline materials, such surfaces are unavoidable. As is the case with grain boundaries, the steps on the surface provide favourable nucleation sites for dislocations and stacking faults, key elements of plastic deformation. We show that deformation mechanisms in copper and nickel are influenced by the presence of steps at the surface.

## 2 EXPERIMENTAL PART

The simulations were performed on an array of substrates, with surface orientations (111), (9 9 11) and (10 10 8). The (9 9 11) and (10 10 8) surfaces are vicinal to (111) and consist of a series of equidistant monoatomic steps that have (001) and (-1-11) oriented microfacets, respectively.

Copper and nickel single crystal thin films of 10 nm thickness were simulated. The simulations of the tensile and compressive uniaxial deformations were performed at 10 K, applying engineering strain at a strain rate of  $\pm 2.5\%$  /ps. The strain direction was perpendicular to the steps.

The boundaries of the simulation boxes were periodic in the *x* and *y* directions and fixed in the *z* direction.

In the  $z$  direction the simulated films were bound by a free surface at the top and by a layer of fixed atoms at the bottom to prevent the loss of atoms at the border of the simulation box and to simulate defect-free bulk. The thickness of this frozen layer was 1.2 nm. These atoms were fixed at the positions they had when equilibrated to 10 K and were remapped at every deformation of the simulation box. All the forces acting on these atoms were otherwise reset to zero.

In the  $y$  direction the size of the simulation box was subject to requirements for periodicity of the terraces and steps for vicinal surfaces. The number of steps and terraces included was 8.

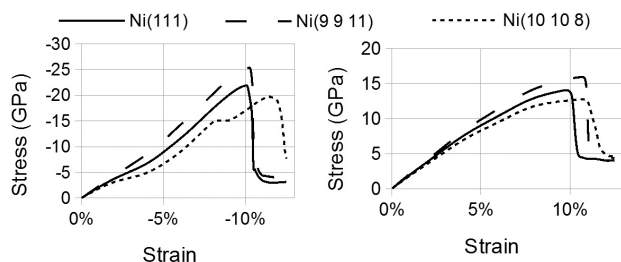
To simulate engineering compressive and tensile strains, the simulation box was deformed in the  $y$  direction in increments of 0.5 % with 200 fs periods of equilibration in-between, resulting in the overall strain rate of 2.5% /ps. The stress in the  $x$  direction was kept to zero.

The molecular dynamics simulations were carried out using the LAMMPS Molecular Dynamics Simulator<sup>9</sup> and EAM potentials by Y. Mishin et al.<sup>10</sup> OVITO<sup>11</sup> was used for visualization and analysis of the simulation data. Dislocation detection algorithm by A. Stukowski<sup>11</sup> implemented in OVITO was used in post-processing.

### 3 RESULTS

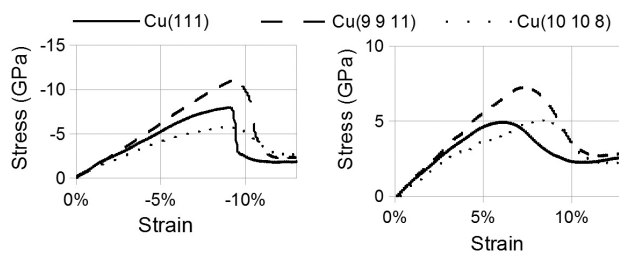
Deformation mechanisms of copper and nickel (111), (9 9 11) and (10 10 8) surfaces were investigated. Stress-strain curves are shown in **Figures 1** and **2**. As is expected from the direction of the strain, the Young modulus (expressed as the steepness of the stress-strain curve) is highest for the (9 9 11) surfaces and lowest for the (10 10 8) surfaces.

Yield stress is lower in copper than in nickel. Both materials exhibit the yield stress asymmetry, with yield stress being higher in compression than in tension. This is connected to the fact that the deformation mechanisms in compression and tension are not the same for any of the surfaces we investigated, although strict geometric analysis suggests otherwise: primary slip systems, namely  $\{-111\}(0-11)$  and  $\{1-11\}(-101)$ , are the same for all the surfaces we investigated, with Schmidt factors of



(a) Nickel, compressive deformation (b) Nickel, tensile deformation  
**Figure 1:** a) Stress-strain curves for nickel deformed in compression and b) in tension.

**Slika 1:** Diagrama napetost-raztezeka za nikelj; a) pri kompresiji, b) pri napetosti.



(a) Copper, compressive deformation (b) Copper, tensile deformation

**Figure 2:** a) Stress-strain curves for copper deformed in a) compression and b) in tension.

**Slika 2:** Diagrama napetost-raztezeka za baker: a) pri kompresiji, b) pri napetosti

0.408 for the (111) surface, 0.377 for (9 9 11) and 0.433 for (10 10 8).

In the case of Cu(111) surface deformed in tension, mostly stair-rod dislocations form throughout the bulk and are not limited to the near-surface region, while in compression, dislocations first nucleate at the surface as Schockley partials and no trailing partials detach from the surface.

In the case of Ni(111) surface deformed in tension, Schockley partial dislocations nucleate in the bulk, while in compression, Schockley partials nucleate at the surface and trailing partials detach from the surface.

For all the (9 9 11) surfaces, Schockley partial dislocation nucleate at the surface and trailing partials detach from the surface. Stair-rod dislocations form in Cu(9 9 11) and Ni(9 9 11) deformed in tension, **Figures 3b** and **3f**.

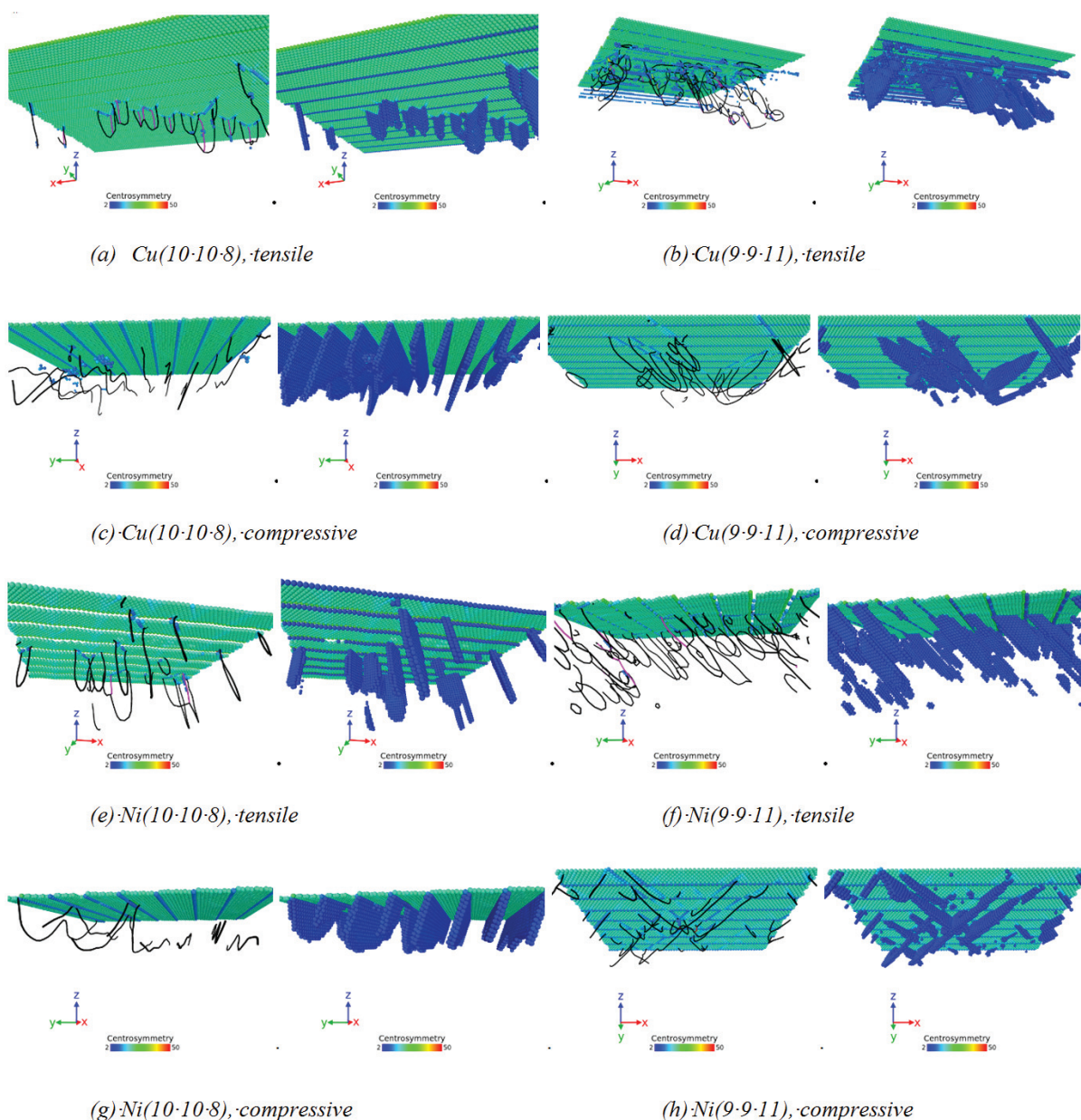
In the case of Cu(10 10 8) surface deformed in tension, **Figure 3a**, stair-rod dislocations nucleate at the surface, while in compression, **Figure 3c**, parallel stacking faults nucleate at the steps and grow into the bulk.

In the case of Ni(10 10 8) surface deformed in tension, **Figure 3e**, Schockley partial dislocation nucleate at the surface and in the near-surface region, while in compression, **Figure 3g**, parallel stacking faults nucleate at the steps and grow into the bulk.

### 4 DISCUSSION

We found two cases of easy glide where only one slip system is active: Cu(10 10 8) and Ni(10 10 8) surfaces deformed in compression, **Figures 3c** and **3g**. Schockley partial dislocations nucleate at all the steps on the surface and grow evenly into the bulk. The stress-strain curves have a small plateau in the region just before the peak of the curve is expected, more pronounced in the case of nickel, and the peak is moved to higher strains, **Figures 1a** and **2a**.

In the case of Cu(10 10 8) deformed in tension, **Figure 3a**, Schockley partial dislocations wrapped around stair-rod dislocations form, also nucleating at the steps on the surface. As the stair-rod dislocations only move with diffusion, which is limited at this temperature, the



**Figure 3:** Dislocation nucleation in copper and nickel thin films deformed in tension and in compression. Two views are shown for each case: dislocations as lines (left) and atoms with centrosymmetry parameter  $CS > 2$  (right). Black lines denote Schockley partial dislocations and pink lines denote stair-rod dislocations.

**Slika 3:** Začetki plastične deformacije v bakrovih in nikljevih stiskanih in raztezanih tankih filmih. Vsak primer prikazujeta dva pogleda: dislokacije označene s črtami (levo) in atomi s parametrom središčne simetrije  $CS > 2$  (desno). Črne črte označujejo Schocklyeve delne dislokacije, roza črte pa Lomer-Cottrell stike.

effect on stress is the same as if only one slip system were active and the stress-strain curve exhibits a change in slope, **Figure 2b**.

A. Zimmerman et al.<sup>12</sup> studied Au(111) surfaces with single monoatomic steps at 0K and found that when the indenter came into physical contact with the step, the deformation mechanism beneath the indenter switched from dislocation emission from the surface to slip aligned with the step.

D. Shan et al.<sup>13</sup> performed a similar study of nanoindentation on thin copper films and found that

when the indenter came into contact with the step, there was a significant difference in the strength of the first dislocation emission.

H. Lu and Y. Ni<sup>14</sup> and H. Lu et al.<sup>15</sup> investigated the effects of surface steps on nanoindentation in Al and found that the shear stress resulting from the step influences the choice of the active slip systems and lowers the threshold for plastic deformation.

Our analysis shows that it is not only the presence of steps that influences deformation mechanisms. While a switch to slip aligned with the steps occurs for the (10 10

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8) surfaces deformed in compression for both materials we investigated, we found no such switch for the (9 9 11) surfaces.

The near-surface region is the first to plastically deform and dislocations nucleate at the surface, therefore the surfaces are softer than the bulk. We conclude that the stress inherent in the steps also lowered the threshold for plastic deformation in our systems.

## 5 CONCLUSIONS

Deformation mechanisms of copper and nickel thin films we investigated are more complex than geometric analysis would suggest. The surfaces are softer than the bulk, as the near-surface region is the first to plastically deform and dislocations nucleate at the surface. We conclude that the stress inherent in the steps lowered the threshold for plastic deformation in the thin films we investigated.

In tensile deformation in both materials, stair-rod dislocations nucleate at the surfaces and are not created by dislocation interactions.

The influence of the surface is most pronounced for the cases of the (10 10 8) surfaces deformed in compression, where parallel stacking faults nucleate at the steps on the surfaces in both materials, overriding the primary slip systems. The presence of the steps does not in itself influence the choice of slip systems. While a switch to slip aligned with the steps occurs for the (10 10 8) surfaces deformed in compression for both materials we investigated, we found no such switch for the (9 9 11) surfaces.

## Acknowledgement

The authors acknowledge the financial support of the Slovenian Research Agency (ARRS).

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