Plastic flow at vicinal surfaces of nickel

Nuša Pukšič, Matjaž Godec, Monika Jenko

Institute of Metals and Technology, Lepi pot 11, 1000 Ljubljana, Slovenia

nusa.puksic@imt.si

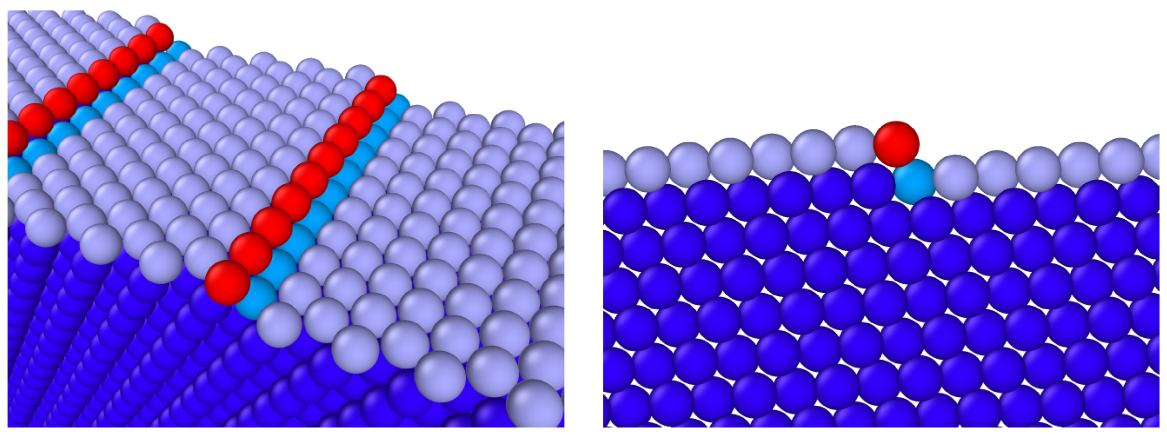
Supplemental videos:

Introduction

Crystalline solids subjected to stresses beyond their elastic limit undergo plastic deformation and subsequently flow. Plastic flow is the continuum description of atomic displacements in a crystalline solid. It involves a wide range of length and time scales, from individual dislocations that move at the nanometer scale to cooperative movement of a large number of dislocations that causes grain boundaries to move at micron scales, ultimately leading to macroscopic response of the solid to applied stresses. In nanoscale materials, atomic-displacement fields are present to a significant degree already in the elastic regime around discontinuities: grain boundaries, precipitates or surface features, namely steps and islands. Through the displacement fields the presence of the discontinuities is communicated into the surroundings. As the density of the discontinuities is high in nanoscale materials, the emergent displacement fields have an effect on the plastic flow. We show plastic flow in nickel thin films with vicinal surfaces, i.e. consisting of equidistant steps, a system appropriate for studying interplay between dislocations and steps.

Vicinal surfaces

Vicinal surfaces consist of equidistant steps divided by low-index terraces. Perspective and side views of a (10 10 8) surface are shown here. Atoms in red are at the step edge, atoms in light blue are in the step corner. The terraces are (111).



Plastic flow

When a crystalline solid is deformed beyond the elastic limit, dislocations form by a collective movement of atoms. Using molecular dynamics, we track the movements of atoms throughout the simulations and can visualize these movements in a series of snapshots.

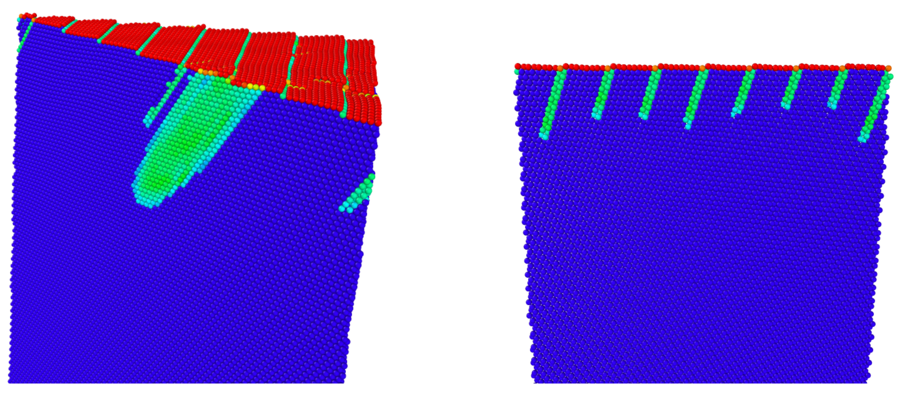
Methodology

Nickel thin films with the surface orientation of (10 10 8) were equilibrated to 10 K, then uniaxially deformed in compression and in tension at a constant strain rate. At this low temperature the diffusion processes and thermal vibrations are suppressed. This reduces noise in the identification of dislocations and visualization of plastic flow.

Periodic boundary conditions were used in the **x** and **y** directions, the simulated slabs had a free surface in the **z** direction and a layer of fixed atoms at the bottom, simulating bulk.

Molecular dynamics simulations were carried out using LAMMPS, postprocessing was done using OVITO.

Results



The above are snapshots from simulations of tensile deformation (left) and compressive deformation (right) of a Ni(10 10 8) surface. The red atoms are the terrace atoms at the surface, the green atoms have slipped, forming dislocations.

Tensile deformation

We will look at the movement of atoms in the plane containing a dislocation. In the left image above, the slice is shown as part of the simulated slab. One dislocation is in the observed plane and we can also see cross-sections of other dislocations perpendicular to the given plane.

Compressive deformation

In compressive deformation, dislocations form parallel to the steps at the surface. We will look at a plane perpendicular to the dislocations as shown above on the right.

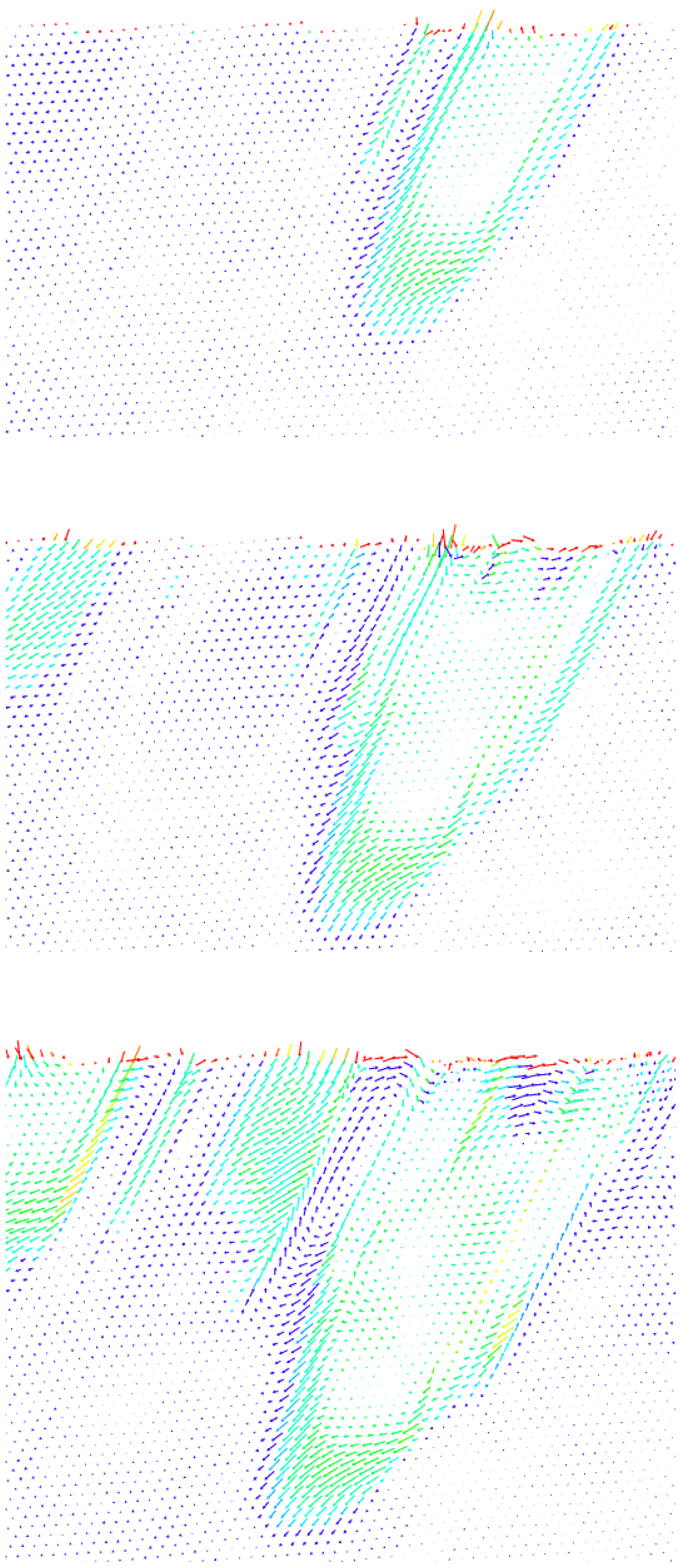
Description

Two sets of three consecutive snapshots are shown. The atoms are represented by arrows that show the direction in which the atoms have moved from the previous snapshot and the length of the arrow is proportional to the displacement, scaled by 4 for better visibility. Red arrows denote atoms at the surface, green arrows denote atoms comprising dislocations.

Conclusions

- In the case of tensile deformation, we find a typical fast decay of displacements of atoms surrounding a dislocation.
- In the case of compressive deformation, the interplay of surface steps and dislocations is observed. Dislocations follow the pattern of surface steps. Displacements of atoms not involved in slip (dark blue) form moving vortices.

Plastic flow in tensile deformation



Plastic flow in compressive deformation