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Influence of the crystallographic orientation and thickness of thin copper coatings during nanoindentation

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ABSTRACT

The structure of interest consists of a nanometer thin copper coating, resting on a stiffer substrate. The elastic and plastic properties of the coating are investigated for three crystallographic orientations and two coating thicknesses using nanoindentation simulated by molecular dynamics. The force–displacement curve, the atomic rearrangement, the stresses and the lattice disorder are monitored during indentation to determine and describe the occurrence and formation of pop-ins and pop-outs during loading. It was found that the crystallographic orientation strongly influenced both the stiffness, load for pop-in formation, the resulting deformation and the stress beneath the indenter.

1. Introduction

The impact of and use in every-day technology from nanosized devices are increasingly important. In the last years nanotechnology has entered as a natural part into a wide range of areas of applications such as medical sensors and nanoelectromechanical systems, NEMS. A frequently occurring part of such a nanodevice is the presence of a nanometer thin coating, with coating properties determined at the atomic level.

It is well known that the mechanical properties of nanosized structures and components differ from those of macroscopic components. This is due to factors such as a low dislocation density, high ratio of number of surface-to-bulk atoms and an increased influence from the crystal orientation; cf. e.g. Olsson et al. [12] or Cuenot et al. [1]. These factors are especially important for thin surface coatings, at the nanometer scale, resting at a relatively thick substrate, cf. Olsson and Melin [13], Hommel and Kraft [5] or Johansson et al. [7].

To be able to design components containing nanometer thick coatings it is important to be able to determine the surface properties of materials on the nanoscale. Today nanoindentation is one of few ways to study and determine the elastic and plastic properties of a material on the nanoscale. The technique corresponds to traditional indentation tests at the macroscopic scale, such as Brinell hardness testing. During a nanoindentation test the force on the indenter and the indentation depth are monitored and a so called force–displacement (P–δ) curve is constructed, covering both the loading and the unloading part of the test. For thin enough coatings, or at large enough indentation depths, the (P–δ) curve can show some irregularities on the otherwise smooth curve during loading, called pop-ins, see e.g. Schuh and Nieh [15] or Nair et al. [11], among others. At such an event the load drops or stays constant, for a short period of time, with increasing indentation depth under displacement control. Pop-in events are generally thought to signal dislocation movements due to different slip events or to sudden crack nucleation. Similar events can also occur during the unloading part of the test, called pop-outs.

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Nomenclature

$\phi_{\alpha\beta}$	pair-wise potential function
ρ_β	contribution to the electron charge density
δ	displacement of indenter
σ_{ij}	per atom stress
ν	Poisons ratio
E_i	potential energy
r_{ij}	distance between atoms
F_α	embedding function
P	force on indenter
R	radius of the indenter
T	coating thickness
W	coating width
uc	unit cell
T	temperature
a_0	lattice parameter
V^α	atomic volume
M^α	atomic mass
v	atomic velocity
$F_i^{\alpha\beta}$	force between atoms α and β
$r_j^{\alpha\beta}$	distance between atoms α and β
CS	centro-symmetry parameter
E	Young's modulus

Several studies on nanoindentation using molecular dynamic (MD) simulations can be found in the literature. Imran et al. [6] studied the influence from the indenter velocity and size of the indenter using MD simulations in Ni single crystals. Nair et al. [11] studied the influence from the indenter radius in thin Ni films and compared it to experimental findings. Also Hansson and Jansson [3] studied the influence on the elastic and plastic behavior of the material due to indenter radius and coating thickness of single crystal copper.

In this paper the influence on the elastic and plastic properties of a thin copper coating due to different crystallographic orientations will be investigated using MD simulations of nanoindentation. The formation of pop-ins and pop-outs in the (P–δ) curve during the indentation process will be investigated as well as what happens in the material at such events. This will be done by studying the atomic rearrangements and by calculating the stress and lattice disorder beneath the indenter during the indentation process.

2. Statement of the problem

2.1. Model geometry

The problem of interest is nanoindentation of a thin copper coating, cf. Fig. 1. Here a spherical indenter with radius of $R = 20$ atomic unit cells (uc), is pushed into a thin copper coating of width $W = 80uc$ and thickness $t = 10uc$ or $t = 20uc$. The thin coating is assumed to rest on an infinitely stiff substrate and three different crystallographic orientations of the coating will be considered and compared. The thin copper coating has a face centered cubic (fcc) structure and the crystallographic directions of the coating are chosen such that the (x,y,z) directions, cf. Fig. 1, coincides with the [100], [010], [001], the [100], [011], [0−11] or the [1−10], [111], [−1−12] directions in the material.

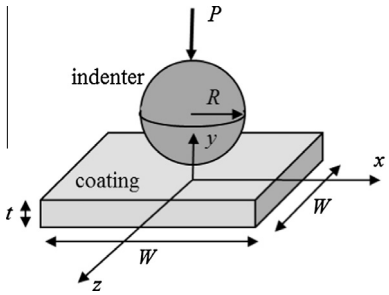

Fig. 1. Schematic description of nanoindentation with a spherical indenter.