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Influence of surface roughening on indentation behavior of thin copper coatings using a molecular dynamics approach

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ABSTRACT

The structure of interest consists of a nanometer thin copper coating, resting on an infinitely stiff substrate and subjected to nanoindentation by a rigid diamond indenter. The elastic and plastic properties of the coating are investigated for different surface roughening position of attack by the indenter using molecular dynamics. The force–displacement curves, the lattice disorders and the stresses are monitored during indentation to determine the onset of plasticity, plasticity development and stiffness in the different cases. It was found that both the surface roughening and point of attack of the indenter strongly affect the elastic and plastic behavior of the thin coating.

1. Introduction

The impact from and use in every-day technology of 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 devices 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 the properties of macroscopic components. This is explained by factors such as a low dislocation density, a high ratio of surface-to-bulk atoms and an increased influence from the crystal orientation at the nanoscale cf. e.g. Olsson et al. [1] or Cuenot et al. [2]. These factors are especially important for very thin surface coatings, at the nanometer scale, cf. Olsson and Melin [3], Hommel and Kraft [4] or Johansson et al. [5].

To be able to correctly design components containing nanometer thick coatings it is important to be able to determine the properties of materials on the nanoscale. Nanoindentation is one of few ways to be able to study and determine elastic and plastic properties of a material at this scale, and this technique corresponds to traditional indentation tests at the macroscopic scale, such as the Brinell hardness test. During nanoindentation the force on the indenter, P, and the indentation depth, δ, are monitored and a force–displacement (P–δ) curve is constructed. For thin enough coatings, or at large enough indentation depths, the (P–δ) curve can show irregularities in the otherwise smooth curve, called pop-ins during loading and pop-outs during unloading, see e.g. Schuh and Nieh [6], Nair et al. [8] or Hansson [9], among others. At such pop-in events the load drops, or stays constant for a short time, with increasing indentation depth under displacement controlled loading, resulting in a drop in the (P–δ) curve. Pop-in events are thought to signal dislocation formation and movement due to different slip events, or to sudden crack nucleation.

Several studies on nanoindentation using molecular dynamic (MD) simulations can be found in the literature. Imran et al. [10,11] studied the influence from the indenter velocity, size of the indenter and crystallographic orientation in Ni single crystals using MD simulations. Nair et al. [8] studied the influence from the indenter radius in thin Ni films and compared the findings to experiments. Hansson and Jansson [12] and Hansson [9] studied the influence on the elastic and plastic behavior of thin Cu coatings due to indenter radius, coating thickness and crystallographic orientation of single crystal copper.

Most previous studies regarding nanoindentation have been performed assuming indentation on a smooth surface. However, for components on the nanometer scale the surface roughening can have a large impact on the mechanical response of the material. Such studies have been performed by Chen et al. [13] in an AISI 316L stainless steel using the finite element method and a Berkovich indenter. Similar studies have also been performed by Bolesta and Fomin [14], among others, using a spherical indenter. When the size of the indenter is of the same order as the surface roughening, the roughening may have a significant effect on the results. Jiang et al. [15] have studied the influence of the indenter radius

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and surface roughening, of the same order of magnitude, in the nanometer range, using a two-dimensional quasicontinuum model of single crystal copper thin film.

In this paper the influence on the elastic and plastic properties of a thin copper coating due to surface roughening and position of attack of the indenter will be investigated through MD simulations of nanoindentation with a spherical diamond indenter. The formation of pop-ins in the (P–δ) curve and the stiffness of the coating will be investigated during the indentation process. Also details about the events taking place within the material regarding defect formation will be monitored and compared to the (P–δ) curve. This will be done by studying both the lattice disorder and the stresses beneath the indenter during the indentation process.

2. Statement of the problem

2.1. Model geometry

The problem of interest concerns the influence of surface roughening during nanoindentation of thin copper coatings. In this investigation a spherical rigid diamond indenter, with radius of $R = 20a_{oCu}$, with a_{oCu} denoting the lattice constant for copper, is pushed into a thin copper coating of width $W = 80uc$ and thickness $t = 20uc$, with uc denoting a copper atomic unit cell, cf. Fig. 1.

The thin coating is resting on an infinitely stiff substrate, where two different surface configurations and four different positions of attack for the indentation will be compared. The first configuration consists of an atomically smooth surface, with no surface irregularities. The second configuration consists of 32 tops and 32 valleys of equal depths $h^* = 2uc$ and widths $b^* = 10uc$, repeated in a regular pattern as described in Fig. 2. The depths and widths of the tops and valleys are chosen so that they correspond to a depth of four atom layers and width of 20 atom layers. The 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 [1 0 0], [0 1 0], [0 0 1] directions of the material.

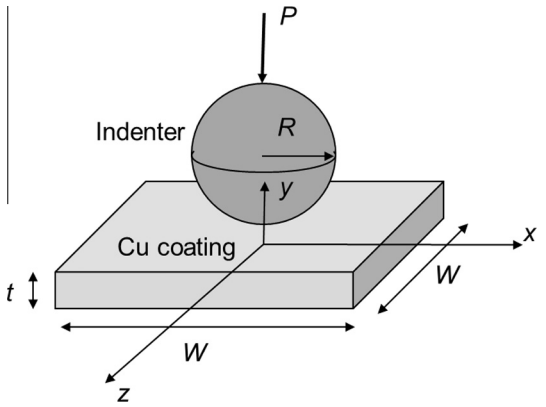

Fig. 1. Schematic description of nanoindentation with a spherical indenter [9].

2.2. Molecular dynamics

To simulate the thin copper coating and the spherical indenter a 3D molecular dynamics approach has been adopted, using the open-source code LAMMPS by Plimpton [16]. The Cu–Cu interaction, within the copper coating, is simulated using an EAM-potential, describing the potential energy of an atom. It consists of one pair-wise repulsive part and one N-body attractive part, with a specific cut-off radii as described in Holian and Ravelo [17]. The potential energy, E_i^α, of atom i of type α is given by Eq. (1).

$$E_i^\alpha = F_\alpha\left(\sum_{i\neq j}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{i\neq j}\phi_{\alpha\beta}(r_{ij}) \tag{1}$$

where α and β denotes two types of atoms, r_{ij} is the distance between atoms i and j, $\phi_{\alpha\beta}$ is a pair-wise potential function, ρ_β is the contribution to the electron charge density from atom j of type β at the location of atom i, and F_α is an embedding function that represents the energy required to place atom i of type α into the electron cloud. In this paper, where the stiff substrate is modelled by cupper atoms restricted from movement, only one type of atoms are modelled using an EAM-potential, meaning that α equals β. In the simulations a potential file given in LAMMPS named Cu_u3.eam, developed by Foiles et al. [18], have been used.

The Cu–C interaction between the indenter and the coating atoms is described using the Morse potential $U_{\text{Morse}}(r_{ij})$, cf. Eq. (2), in accordance with Zhang and Tanaka [7] and Pei et al. [19], with parameters D, α and r_0 according to [7] as shown in Table 1.

$$U_{\text{Morse}}(r_{ij}) = D[e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}] \tag{2}$$

The indenter is treated as infinitely stiff, not allowing movement of the carbon atoms. Therefore no potential for the C–C interaction is necessary, an approach also used by Liang et al. [20], among others. In this paper also the substrate beneath the thin copper coating is treated as infinitely stiff. This is modelled by restricting the bottom atomic layers of the coating from movement in all directions. Further, periodic boundary conditions have been employed in the x- and z-direction, cf. Fig. 1, thus simulating an infinitely large thin coating. The atomic gitter with a rough surface,

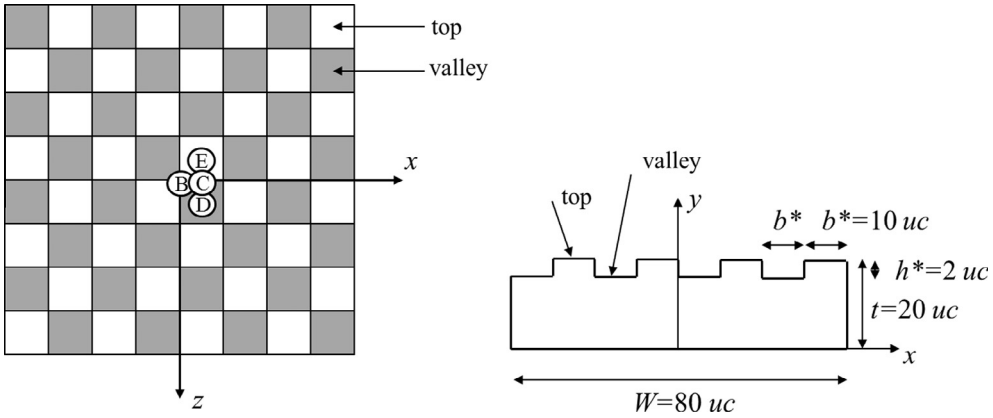

Fig. 2. Schematic description of the surface roughening and the placement of the center of the indenter.