Surface roughness of gold substrates at the nanoscale: An atomistic simulation study

Soheil Solhjoo, Antonis I. Vakis

PII: S0301-679X(17)30261-X

DOI: 10.1016/j.triboint.2017.05.024

Reference: JTRI 4743

To appear in: *Tribology International*

Received Date: 15 February 2017

Revised Date: 25 April 2017

Accepted Date: 16 May 2017

Please cite this article as: Solhjoo S, Vakis AI, Surface roughness of gold substrates at the nanoscale: An atomistic simulation study, *Tribology International* (2017), doi: 10.1016/j.triboint.2017.05.024.

Surface roughness of gold substrates at the nanoscale: an atomistic simulation study

*Soheil Solhjoo, and Antonis I. Vakis**

Advanced Production Engineering, Engineering and Technology Institute Groningen, Faculty of Science and Engineering, University of Groningen, Nijenborgh 4, 9747 AG Groningen, the Netherlands

**Corresponding author: a.vakis@rug.nl; +31 50 363 4202*

Abstract

The statistical properties of rough surfaces at the nanoscale are studied using classical molecular dynamics. Atomistic fcc blocks of gold are generated with different crystal orientations, and with rough surfaces having the same root-mean-square roughness with variable power spectral density (PSD) slopes and roll-off wavenumbers. The process of rough surface generation may result in thermodynamically unstable sharp spatial features. In order to relax the structure, the blocks are equilibrated at $300\ \mathrm{K}$. It is found that all surfaces experience changes in their roughness, regardless of their crystal orientation or temperature, although the changes are only temperature-independent when $T \leq 0.4T_{\mathrm{m}}$. Based on the analyzed PSDs of the equilibrated substrates, two methods for generating pseudo-stable rough surfaces are introduced and discussed.

Keywords: nanoscale, surface roughness, atomistic models, classical molecular dynamics.

1. Introduction

As a consequence of the miniaturization of mechanical devices, a large number of tribological research studies have been directed toward the atomic scale. Due to the limited lateral resolution of measuring devices in comparison to atomic spacing, researchers utilize atomistic computer simulation methods, e.g. classical molecular dynamics (MD), in order to investigate different tribological processes, such as normal or frictional contacts. In these works, the substrate is usually represented, either, as a flat or a simple patterned surface. One can also find a limited number of tribological MD studies which employed randomly rough substrates [1-12]; however, due to limitations in the lateral resolution of measuring devices, the nature of the atomic-scale roughness present on real surfaces is still under question. An important result stems from the work of Oliver et al. [13] who studied the morphology of tungsten nanoparticles using field-ion microscopy, and showed they have a stepped geometry; this was later used