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## Molecular dynamics and experimental study on comparison between static and dynamic ploughing lithography of single crystal copper

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### Abstract

Dynamic ploughing lithography based on atomic force microscope (AFM) is a promising technique for fabrication of nano structures and devices. This study investigates the material removal mechanism and surface generation in dynamic ploughing of single crystal copper by molecular dynamics (MD) simulations in addition to the experimental tests, and compares it with that of static ploughing lithography. It is found that the material removal in dynamic ploughing is mainly due to downwards and sideways slipping of workpiece material on the {111} slip planes and the subsequent elastic recovery, whereas forwards and sideways slipping account for the material removal in static ploughing. As a result, there is little chip formation in dynamic ploughing, while significant chip formation is observed for static ploughing in both simulations and experiments. In addition, this results in smaller groove depth and width for dynamic ploughing, allowing fabrication of nanostructures with smaller features. The slipping processes in both static and dynamic ploughing can be corresponded with the periodical variations of machining forces. The average machining force in dynamic ploughing is significantly smaller than that in static ploughing. This indicates the possibility of reducing the wear of AFM tip by employing dynamic ploughing lithography, since the tip wear is greatly influenced by the magnitude of machining force. These results reveal the mechanism of material removal and surface generation in dynamic ploughing lithography, which can be of useful reference for its practical application in nanomanufacturing.

**Keywords:** Atomic force microscopy; Static ploughing lithography; Dynamic ploughing lithography; Single crystal copper; Surface generation

### 1. Introduction

Recently, nanoscale structures have attracted more and more attentions in various fields, such as nano optics, micro/nano sensors and micro/nano electromechanical systems [1-3]. There are various approaches to fabricate nanoscale structures with high accuracy, including electron beam lithography (EBL) [4], focused ion beam (FIB) lithography [5], and nanoimprint lithography (NL) [6]. However, their applications are greatly impeded by the disadvantages of complex operation, strict environmental

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