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Mechanism of material removal during nanofinishing of aluminium in aqueous KOH: A reactive molecular dynamics simulation study

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ABSTRACT

In this work, the atomic mechanism of tribo-chemical wear of aluminium at the interface of Si—Al in aqueous KOH environment was investigated using a reactive molecular dynamics simulation (R-MDS) for achieving nano-finished surface using the principle of chemically assisted mechanical finishing (CMAF) through chemo mechanical magnetorheological finishing (CMMRF) process. Three attributes of material removal mechanisms were detected in the finishing process. The first is caused by the destruction of parent bonds on the aluminium substrate surface and is assisted by the oxidation. The second is caused by the mechanical stress assisted chemical reaction to bridge new bonds between abrasive and workpiece. The third is caused by rupture of Al—Al bonds, as the newly formed bonds are relatively strong. This work shows that the removal of Al atoms from the substrate is a result of both chemical reaction and mechanical effects, and contributes to the understanding of tribo-chemical wear behaviour of CMMRF process. The finished surface shows free of any other contamination which is suitable to employ such surfaces for the micro-electronics fabrication. Experimental results also support the mechanism of CAMF for generating the surface finish of the order of few nanometers.

1. Introduction

Nanofinishing is an essential process of manufacturing technology, which helps to cater the requirements of high precision components in various fields of engineering such as optical, micro-mechanical, micro-electronics and bio-medical. There are many engineering materials which are segregated on the basis of their physical, chemical, electrical, mechanical and optical properties to serve the functional attributes of parts.

In case of integrated circuits (ICs) and optics, some essential parameters need to be maintained like high conductivity, low mass density, high corrosion resistance, optical reflectivity etc. To maintain such properties, aluminium alloy was widely used in micro-fabrication, Gamma ray's telescope, adaptive optics, optical sensors, microelectronic devices [1–3] and very large scale integration for conductive wires [4]. However, Aluminium possesses ductility, malleability and poor resistance to scratching [5] behaviour as mechanical properties which introduce challenges for generating nanometric surface finish by using abrasive based finishing process. To overcome such problem, few experimental works are carried out in the field of CMP [6] and CMMRF [7,8] processes for nanofinishing of aluminium alloy. These processes work on the principle of chemical reaction followed by mechanical abrasion which can also be called as chemically assisted mechanical finishing (CAMF).

During such CAMF process, the chemical reactions get accelerated by mechanical forces applied through the abrasive particles [9]. In general, slurry for finishing of aluminium workpiece contains alkaline medium, which forms aluminium hydroxide during the process and it can speed up material removal as well.

With the development of ICs and optical industries, the chemically assisted mechanical finishing for CMP and CMMRF technologies need to achieve the nanometer or angstrom level roughness without damaging the surface, which is an extreme limit of the surface engineering. Hence, it is essential to understand the mechanism of material removal during the chemically assisted mechanical finishing of aluminium as workpiece material.

Since, the experimental studies at macroscale of CMP and CMMRF are not suitable to understand the combined effect of chemical reactions

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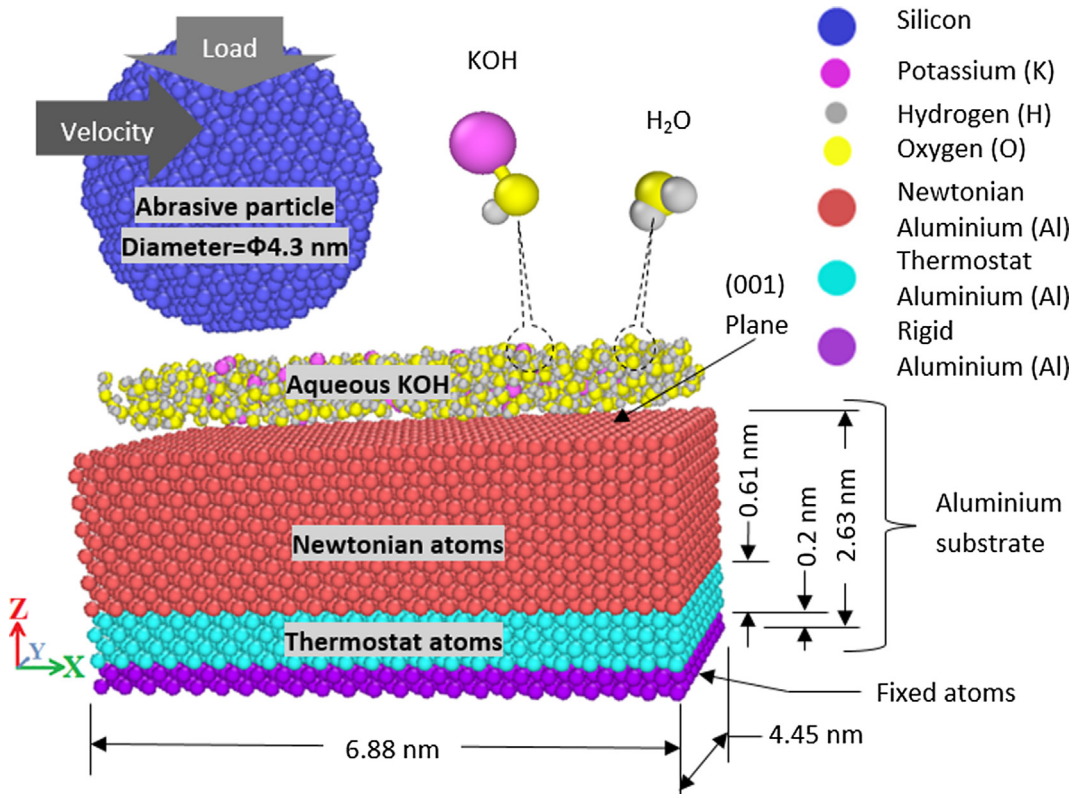

Fig. 1. Schematic diagram of the model for reactive MD simulation of Al-nanofinishing in the aqueous KOH. Size of MD simulation cell = 6.88 nm × 4.45 nm × 8 nm.

and mechanical abrasion, of process parameters at nanometric scale. Moreover, experimental study by means of atomic force microscope cannot reveal the details about the dynamic aspects of nanofinishing, thus the experimental technology is unable to illustrate the process mechanisms in-depth. In order to understand the combined effect of chemical reactions and mechanical effects in this dynamic process, molecular dynamics simulation (MDS) has become an easy and efficient tool.

As far as molecular dynamics (MD) simulation is concerned, it is categorised in two main classes, i.e. Classical molecular dynamics simulations based on empirical force fields, and other is known as quantum chemical (QC) MD simulation which works on basis of ab-initio MD simulation in which Schrodinger wave equation is solved with suitable approximation method to generate accurate results. Classical MD simulation technique is suitable to study mechanical abrasion in reasonable computation effort. QC-MD simulation is suitable for chemical study, which takes excessive computation effort as compared with classical MD simulation. To overcome the demerits of classical and QC-MD simulation another method was developed to simulate both chemical reactions and mechanical effects at the same time and comparatively reasonable computational effort, and this method is called as reactive MD simulation. Reactive MD simulation works on the principle of reactive force field (ReaxFF) which is developed by fitting a large set of data generated from the QC simulation. In general, ReaxFF includes various functions of energy as a set of parameters such as bond energy, atom energy, lone-pair energy, molecule energy, valence angle energy, double-bond valence angle penalty, valence angle conjugation energy, hydrogen bond energy, torsion energy, conjugation energy, van der Waals energy, Coulomb energy, electric field energy, and charge equilibration energy [10]. Hence, this technique is favourable for simulating chemical reactions and mechanical attributes of the chemical assisted mechanical finishing process.

In the present work, a reactive force field based MD simulation is carried out to study the CAMF based nanofinishing process on aluminium workpiece under the presence of aqueous KOH and silicon abrasive particles. The details of computational aspects of MD simulation are described in the next section. Results of simulation are also discussed with the mechanism of material removal at atomic scale. In addition, experiments are also conducted to understand and verify the capabilities of CAMF based process through CMMRF process.

2. Methods and models

2.1. ReaxFF method

In general, quantum chemical (QC) techniques are worthwhile for chemical systems, which perform quantum chemical calculation based on electronic level (such as Schrodinger wave equations of electrons). Hence, it makes computationally expensive or inapplicable for large (say, more than100 atoms) systems. QC methods are also known as quantum mechanical molecular dynamics simulation. Classical molecular dynamics simulation employs empirical force field (EFF) methods in which the relationship between energy and geometry is a set of fairly simple potential functions to simulate much larger systems than QC systems, e.g., thousands of atoms on single processors, and millions of atoms on multiprocessors. However, EFF methods are only trained for systems in which the bonds remain within about 75% of their equilibrium value. For this reason, EFF methods cannot describe reactive systems.

Reactive force field (ReaxFF) is a sophisticated technique to compute the forces between atoms developed to bridge the gap between QC and EFF based computational methods of molecular dynamics simulation. Thus, the ReaxFF method has an additional capability for the computation of chemical reaction which allows chemical bond to break and form.

To describe the various interaction among aqueous potassium hydroxide and aluminium surfaces during nanofinishing process, optimization of the force field is essential to acquire proper parameters values.