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MD simulation study to investigate nanocutting process in Cu and CuBe

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Abstract

Impurities and inhomogeneity in the metallic materials change the material deformation and removal mechanisms drastically based upon the impurity content in them. Even a small percentage of Be (0.5-2%) addition in Cu alters the mechanism involved in the cutting process significantly. Since it becomes experimentally difficult to observe the mechanisms involved in the nanocutting process due to its length scale, molecular dynamics simulation provides deep insights during cutting process considering the discrete effects of material. Therefore in this study molecular dynamic simulation (MDS) of cutting operation was performed on Cu and CuBe assuming Cu as single crystal in both the cases. Results show that Be particle in Cu affects the material deformation and cutting forces significantly. It is observed that dislocation flow is obstructed by the particle and tool shows wear at the cutting edge in the form of chipping.

Keywords: Nanocutting, diamond turning, cutting mechanism, tool wear.

1. Introduction

Ultraprecision machined Cu and its alloys are widely finding applications in the area of laser optics and electronics industry. CuBe is popular material which is used as window material in infrared applications. Usually single point diamond turning is employed to generate highly finished surface in the range of few nanometers with shape and size accuracies of the order of nanometers [1]. Cutting edge sharpness of the order of few nm enables material removal in a very small cutting zone and generates smooth surface. However, presence of impurities distort the continuity of workpiece material and also affect the cutting process in terms of surface quality and tool condition.
Very limited research has been carried out in nanocutting of workpieces with presence of impurities. Li et al. (2016) studied the effect of pores and second phase particles on the subsurface damage, surface integrity. They linked the presence of pores to work hardening and presence of particle to low subsurface damage [2]. Xu et al. (2017) considered diamond as a hard particle in Al workpiece and showed that its presence affects the deformation and surface integrity [3].
Be in Cu exists as hard particle and affects the material deformation and surface generation and excessive tool wear is also observed. However, mechanism of material removal and wear during tool and hard particle interaction have received little attention. Experimental techniques at such small cutting scale becomes redundant to observe the mechanisms. Therefore the present study involves the molecular dynamics simulation to investigate tool and workpiece interaction in both Cu and CuBe to understand the effect of presence of hard particle in the cutting process. Section 2 contains details of atomistic model of tool and workpiece. Section 3 discusses about results and discussions. Section 3.1 and 3.2 . Section 4 concludes the study carried out in this paper.

2. SIMULATION METHODOLOGY

2.1. Cutting simulation geometry and conditions

Fig. 1 shows the MD model of tool and workpiece employed for both Cu and CuBe. CuBe comprise of Be particle in Cu base material. The computational parameters used in MD simulation are presented in Table 1. Both the tool and workpiece comprised of three layers viz. Newtonian layer, thermostat layer and boundary layer. Periodic boundary condition (PBC) was applied to the z-direction in order to reduce the size effects and realize the bulk material conditions.

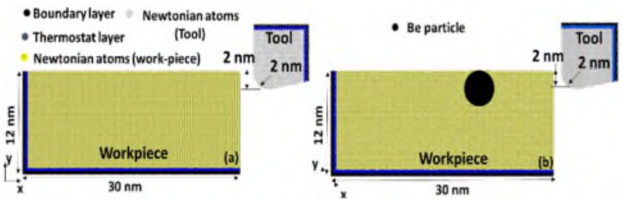

Figure 1. MDS model for nanoscale cutting of (a) Cu (b) CuBe

Table 1 Computational parameters used in MDS of nanoscale cutting.

Workpiece material	Cu & CuBe
Cutting plane and direction	(010)[100]
Dimensions	30 nm x 12 nm x 18.15 nm
Tool (Deformable)	Single crystal diamond
Cutting edge radius (R)	0 and 20 Å
Uncut chip thickness (a)	20 Å
Cutting velocity	1 Å/ps
Equilibration Temperature	293 K
Time step	0.001 ps

2.2. Choice of Potential Energy function:

Cu has face centered cubic (FCC) lattice structure and interaction between the copper atoms is precisely expressed by Embedded Atom Method (EAM) potential [4]. EAM potential is expressed by the following equation:

$$U_{tot} = \frac{1}{2}\sum_{j\neq i} V(r_{ij}) + \sum_{i} F_i(\rho_i) \qquad (1)$$

Where V denotes a pair potential. F_i designates embedding energy that represents the energy to place an atom i in a host electron density (ρ_i) at the site of that atom i, induced by all other atoms in the system. Diamond (sp3 bonded Carbon) consists of diamond cubic structure in which atoms are bonded together with covalent bonds. A 3-body potential based on ABOP formalism was used to describe the C-C interaction [5]. Total energy using ABOP function is a sum over each bond energies:

$$E=\sum_{i>j} f_c(r_{ij})\left[V_R(r_{ij})-\frac{b_{ij}+b_{ji}}{2}V_A(r_{ij})\right] \quad (2)$$

Where E is the cohesive energy which is the sum of individual bond energies which has following pairwise repulsive and attractive contributions.

Morse pair potential function was used to describe interaction of Be and C atoms with Cu atoms. Morse potential function [6] is expressed by Eq. 3.

$$V(r_{ij}) = D[\exp(-2\alpha(r_{ij}-r_o)) - 2\exp(-\alpha(r_{ij}-r_o))] \quad (3)$$

Where, D, r_{ij}, r_0 and α are the binding energy, arbitrary distance between i and j atoms and equilibrium atomic spacing, elastic modulus respectively.

3. Results and discussion

Cutting in Cu and CuBe shows the flow of dislocations due to deformation caused by forces imposed by the tool in the material. Cutting action causes stacking faults in Cu which propagate with the tool movement in cutting direction as shown in Fig. 2. It can be observed that the dislocations flow ahead and below the tool due to normal force owing to edge roundness. However Be particle in CuBe resists the dislocations to flow when tool starts approaching particle. Particle being hard in nature, it itself starts cutting the base material and lot of deformation in the form of dislocations flow take place with dislocations loops gliding into the material as shown in Fig. 3. Dislocation reduces first in CuBe, and then increase significantly as shown in plot in Fig. 4. After tool and particle interaction, dislocation density decreases.

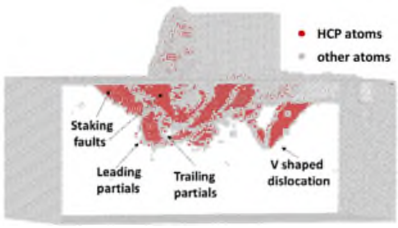

Figure 2. Nano cutting of Cu

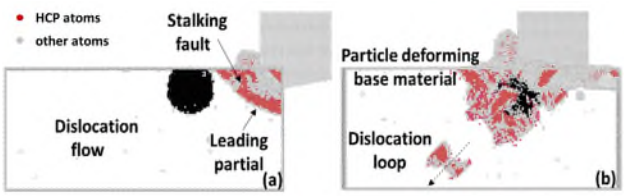

Figure 3. Nano cutting of CuBe at (a) initial phase (b) particle location

Deformation during cutting cause subsurface damage under the machined surface which in practice affects the optical as well metallurgical properties. Subsurface damage observed during cutting in CuBe is significantly higher than that of Cu. It is noticed to be 10nm in CuBe as compared to Cu where it is 3.5 nm. Higher subsurface damage in CuBe takes place due to increase in dislocations formation and expansion in the base material owing to particle induced deformation.

Cutting forces alter due to change in cutting action owing to the presence of hard particle. Cutting Cu shows a uniform increase in resultant force, however in case of CuBe, resultant force shows significant jump in value. This is due to the fact that hard particle resists cutting action. Due to the sudden change in cutting force, tool suffers an impact and large stresses at cutting edge which abrade the tool edge. Cu does not show any sign of wear as it is a soft material and smooth cutting action occurs.

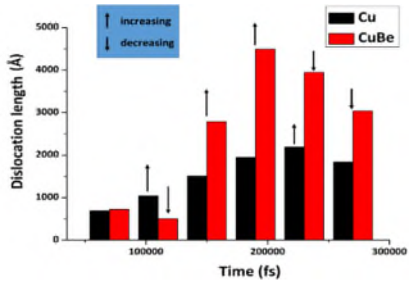

Figure 4. Dislocation evolution during cutting of CuBe

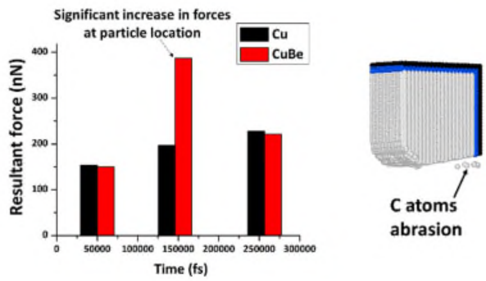

Figure 5. Cutting forces in Cu & CuBe and tool edge degradation in CuBe

4. Conclusions

The study comprises nanocutting of Cu and CuBe and influence of hard particle is investigated on material deformation as well as on cutting tool. Molecular dynamics simulation was applied to understand the phenomena of material removal and deformation in addition to tool edge wear. Based on this study, following conclusions are made:

1. Presence of hard particle in Cu increases the subsurface damage approx. 2-3 times.
2. Cutting forces increase at hard particle location significantly which abrade C atoms from tool edge.

This work leads to understanding of the phenomenon during nanocutting in the workmaterial which contains defect or impurities. Since the present work contain only single impurity as hard particle in the workpiece, further study can be aimed at considering more no. of particles and of different sizes.

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