

Full Length Article

Nanometric mechanical cutting of metallic glass investigated using atomistic simulation

Cheng-Da Wu^a, Te-Hua Fang^{b,*}, Jih-Kai Su^b^a Department of Mechanical Engineering, Chung Yuan Christian University, 200, Chung Pei Rd., Chung Li District, Taoyuan City 32023, Taiwan^b Department of Mechanical Engineering, National Kaohsiung University of Applied Sciences, Kaohsiung 807, Taiwan

ARTICLE INFO

Article history:

Received 3 August 2016

Received in revised form

27 September 2016

Accepted 22 October 2016

Available online 22 October 2016

Keywords:

Metallic glass

NiAl

Cutting

Molecular dynamics

ABSTRACT

The effects of cutting depth, tool nose radius, and temperature on the cutting mechanism and mechanics of amorphous NiAl workpieces are studied using molecular dynamics simulations based on the second-moment approximation of the many-body tight-binding potential. These effects are investigated in terms of atomic trajectories and flow field, shear strain, cutting force, resistance factor, cutting ratio, and pile-up characteristics. The simulation results show that a nanoscale chip with a shear plane of 135° is extruded by the tool from a workpiece surface during the cutting process. The workpiece atoms underneath the tool flow upward due to the adhesion force and elastic recovery. The required tangential force and normal force increase with increasing cutting depth and tool nose radius; both forces also increase with decreasing temperature. The resistance factor increases with increasing cutting depth and temperature, and decreases with increasing tool nose radius.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

Metallic glasses (MGs) are a promising class of materials for advanced applications in engineering, such as microelectromechanical systems [1], functional films [2], and nanomolds [3,4], due to their unique physical properties, such as high mechanical strength and hardness, high toughness, good corrosion resistance, minimal shrinkage, and low friction [5–8]. MGs are metallic alloys with no long-range atomic order (i.e., they have an amorphous structure) and lack the typical defects found in metals, such as dislocations and grain boundaries [9]. The physical properties of MGs are thus completely different from those of crystalline metals.

Casting technology has been widely used for the fabrication of MG components, but the control over dimensional precision and surface roughness of a casting are still not ideal; in addition, the presence of internal defects can even reduce mechanical strength. Mechanical cutting is an alternative for machining complex three-dimensional surfaces in a controllable way with a nanometric surface finish and submicron geometric accuracy [10,11]. Mechanical cutting produces much heat and plastic deformation on a

workpiece surface. For MGs, the shear transformation zone (STZ) is considered as the fundamental unit of plastic deformation, which is a point defect with high stress concentration. Hodge et al. [12] investigated the abrasive wear of Zr, Pd, Cu, and La-based MGs using nanoindentation. They found that the scratched surfaces were significantly different for MGs with different compositions, and that their wear resistance did not follow the classical Archard equation. Huang et al. [13] performed nanoscratch experiments on four bulk MGs and found that a high hardness produces good scratch resistance, which was found to depend on scratch velocity. Overall, the deformation mechanism of MGs is still not completely understood. Molecular dynamics (MD) simulation is a powerful tool for studying material interaction at the nanoscale and its mechanics. Atomic simulation avoids experimental noise and can reduce cost. Many nanosystems related to mechanical manufacturing have been analyzed using MD, such as nanoforming [14,15], nanoscratching [16], nanodrilling [17], and nanomilling [18].

The purpose of this work is to study the cutting mechanism and mechanics of an amorphous NiAl workpiece utilizing MD simulation. The effects of cutting depth, tool nose radius, and temperature on the amorphous NiAl workpiece are studied. The results are discussed in terms of atomic trajectories and flow field, shear strain, cutting force, resistance factor, cutting ratio, and pile-up characteristics.

* Corresponding author.

E-mail addresses: nanowu@cycu.edu.tw (C.-D. Wu), fang.tehua@msa.hinet.net (T.-H. Fang), yummy_2468@yahoo.com.tw (J.-K. Su).

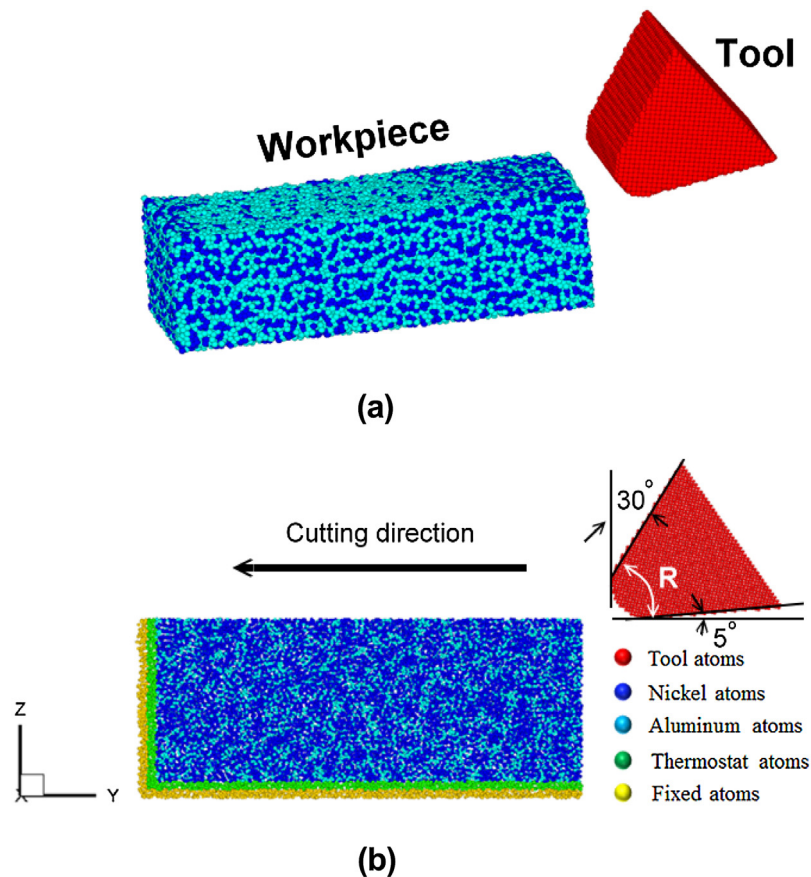


Fig. 1. (a) Schematic of three-dimensional cutting model of amorphous $\text{Ni}_{50}\text{Al}_{50}$ workpiece. (b) Two-dimensional cutting model. Cutting tool is made of diamond and has clearance angle of 5° and rake angle of 30° .

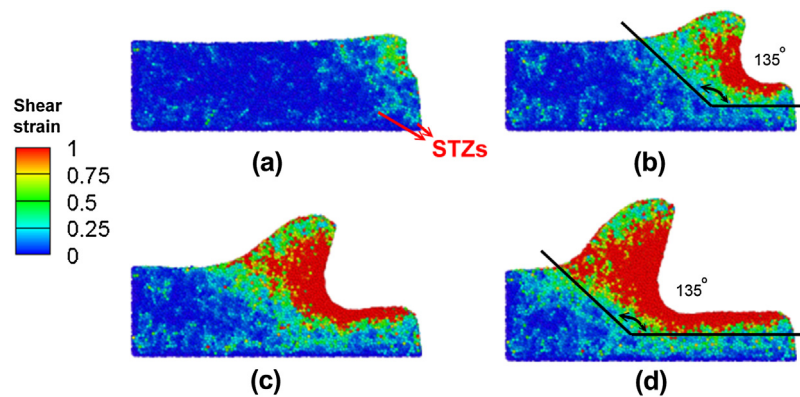


Fig. 2. Snapshots of cutting process of workpiece (tool not shown) at $D = 3.0$ nm and temperature of 300 K for cutting distances of (a) 2, (b) 5, (c) 8, and (d) 11 nm. Workpiece atoms are colored according to magnitude of their shear strains. Chip formed with shear plane of 135° .

2. Model and methodology

The structure of an amorphous $\text{Ni}_{50}\text{Al}_{50}$ workpiece at a temperature of 300 K was obtained from a melting and quenching simulation. The $\text{Ni}_{50}\text{Al}_{50}$ workpiece was initially arranged as a body-centered cubic structure (B2 structure). The isobaric-isothermal ensemble (NPT) and the Nosé-Hoover thermostat were used. The simulations were carried out under three-dimensional periodic boundary conditions (PBCs), and the external pressure was maintained at zero. The workpiece was heated from 300 to 1750 K at a constant heating rate of 0.5 K/ps, obtaining a liquid state from the solid, followed by thermal equi-

librium at 1750 K for 75 ps. Finally, the workpiece was cooled from 1750 to 300 K at a high cooling rate of 5 K/ps and then equilibrated at 300 K for 75 ps.

The physical model of the cutting process for the amorphous NiAl workpiece consists of a diamond tool and an amorphous NiAl workpiece, as shown in Fig. 1(a) and (b). The whole tool was assumed to be an ideally rigid object to simplify the cutting problem and focus on the deformation of the workpiece. The rake angle and clearance angle of the tool were set to 30° and 5° , respectively, for promoting chip flow and decreasing the contact area between the tool and the workpiece. The tool thickness was 7.4 nm. The workpiece dimensions were 7.4 nm (X) \times 21 nm (Y) \times 6.5 nm (Z).

Download English Version:

<https://daneshyari.com/en/article/5352710>

Download Persian Version:

<https://daneshyari.com/article/5352710>

[Daneshyari.com](https://daneshyari.com)