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Nanotribological properties of bulk metallic glasses

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ABSTRACT

Bulk metallic glasses (BMGs) exhibit unique mechanical properties; however, a detailed understanding of nanotribological properties of BMGs is still lacking. In this article, alloy composition, surface disorder, normal load, and velocity dependence of friction between a single asperity contact and the BMG surface is explored with two-dimensional Prandtl-Tomlinson (PT) model. Our numerical results reveal distinct regimes for load and velocity dependence of friction at small length scales. The friction is inert to alloy composition and surface roughness for small loads in wearless regime. Surface corrugation increases with the number of alloy elements and dominates the friction for normal loads that may lead wear. Calculations for the effect of sliding velocity on friction between a single-atom contact and different BMGs show that velocity dependence of friction is inert to alloy composition and surface structure for sliding velocities smaller than 1.3 μm/s. Besides, the friction evolves non-monotonically with alloy composition and surface disorder for larger sliding velocities. Our numerical results show that tracking the minimum energy path and slip-stick motion determine the nanotribological properties of BMGs. The single asperity can trace the minimum energy path at small loads and sliding velocities while increasing load and sliding velocities impede following the minimum energy path with inflation in slip-stick motion. Our analyses disclose that BMGs unveil two unique frictional properties at small length scales: (I) friction is inert to alloy composition and surface disorder in wearless friction regime, (II) velocity dependence of friction does not depend on composition and disorder for small sliding speeds. These results promote BMGs as ideal materials for applications that require high durability and low friction in quasi-dynamic operating conditions.

1. Introduction and background

Bulk metallic glasses (BMGs) are multicomponent alloys with glass structure as crystallization is impeded upon cooling [1,2]. At least two metallic elements are required to formulate BMGs, while one metallic element can form BGMs with metalloids and nonmetals [3–7]. The structure of BMGs does not reveal any long-range order, and the short-range order is characterized by a random distribution [6,8,9]. The deformation characteristics of BMGs are different than their crystal counterparts and exhibit outstanding mechanical properties [10–15]. Similar to metals, frictional properties of BMGs are linked to material hardness [16]. Experiments show that macroscopic frictional properties of metallic glasses are associated with wear, oxidation, temperature, and relaxation [17–25]; however, a detailed analysis to explore the effect of alloy composition, surface disorder, normal load, and velocity on frictional properties of BMGs at small length scales is still lacking.

Friction is an interface phenomenon and is one of the oldest concepts in physics due to its scientific and technological importance [26,27]. After Leonardo da Vinci conducted first systematic studies on friction [28,29], Guillaume Amontons and Charles Augustine Coulomb dictated laws of macroscopic dry sliding friction [30,31]. According to Amontons and Coulomb, friction is proportional to normal load, independent of the contact area, and sliding velocity. These three laws have been used to describe the macroscopic dry sliding friction for centuries; however, revealing the frictional properties of microscopic bodies still remains a challenge [32–37]. Experimental tools such as the surface force apparatus [38], quartz crystal microbalance [39], and lateral force microscope [40] enable characterization of friction down to the nanoscale. Experiments and theoretical work addressed that laws of macroscopic friction collapse at small length scales, i.e. friction evolves with the contact area and the relative velocity between sliding contacts [34,35,37,41,42]. Due to contact area dependence of friction at nanometer length scale, the frictional properties of a single asperity contact have to be explained in order to disclose the friction in complex macroscopic systems [34,35,43,44]. Lateral force microscopy, an extension of scanning force microscopy [45], is the ideal platform to probe nanotribological properties of the interface between a single atom and a surface [32,34,46]. The interaction of the point contact with

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a surface can be described with well-established Prandtl-Tomlinson (PT) model [33,40,41,47–57]. In this article, we investigate the frictional properties of BMGs as a function of alloy composition, surface structure, normal load, and velocity with two-dimensional PT model.

Our numerical results disclose that although binary and ternary alloys have larger surface corrugation, the friction between the single-atom probe and the BMG surface has only saddle differences compared to unary crystals and random unary surfaces in wearless friction regime. Surface disorder increases with the number of alloy elements and dominates the friction for large normal loads that may induce wear. Our results for the velocity dependence of friction for BMGs address that friction is inert to alloy composition for velocities smaller than 1.3 μm/s. Friction displays a non monotonic trend with composition with increasing sliding velocities. Our numerical results reveal that tracking the minimum energy path and the slip-stick motion are two competing effects that dominate the load and velocity dependence of friction for different BMGs. The single asperity can track the minimum energy path for small loads and sliding velocities; however, with increasing load and sliding velocity, the slip-stick motion inflates and leads an increase in friction by inhibiting the tracking minimum energy path. To summarize, our theoretical analyses report that BMGs display unique frictional properties: (I) friction has a weak dependence on surface corrugation and alloy composition in wearless friction regime, (II) velocity dependence of friction is inert to composition for small sliding speeds. These results endorse BMGs for applications that require high durability and low friction under quasi-dynamic operating conditions.

2. Methods

Hölscher et al. developed a two-dimensional model based on PT model for the interaction of a single-asperity with the surface, which has been implemented successfully to explain the atomic scale friction as a function of normal load and velocity [33,36,51,56,58,59]. In a recent article (Ref. [59]), we explored the differences for the predictions of one-dimensional and two- dimensional PT models for load, velocity, and surface disorder dependence of friction. In this article, we apply two-dimensional PT model to different BMG structures.

We used 6–12 Lenard-Jones potential to model the local interaction between the single-atom contact and the model surface in our calculations [60]:

$$V_{L-J} = 4 \epsilon \, [(\sigma/r)^{12} - (\sigma/r)^{6}] \quad (1)$$

In Eq. (1), r denotes the distance between the centers of two atoms, ϵ is the depth of potential well and σ is the distance at which the potential well vanishes ($\sigma = d/1.12$, where d is the hard sphere diameter of the atom). The simulation cell is a 5-atom thick slab with a cross-section of 33 × 33 atoms with periodic boundary conditions along lateral directions (*See* Fig. 1 *for further details*). For binary, ternary, and quaternary alloy systems, we randomly selected the type of the element for each lattice position, which lead the same ratio of elements in alloy compositions, i.e. binary ($A_{50}B_{50}$), ternary ($A_{33}B_{33}C_{33}$), and quaternary ($A_{25}B_{25}C_{25}D_{25}$). Also, we imposed the disorder by adding a random displacement to the unperturbed lattice up to 15% of the diameter of the element along orthogonal directions (x, y, and z). Although more advanced rendering techniques for kernels are available [6], we implemented this simple approach to reduce the computational cost of successive calculations and to have a relative variation for frictional properties of disordered alloy compounds rather than finding the exact friction coefficients. We set the ratio of diameters as 0.8 for different alloy compounds [5,61]. We scaled parameters for the interaction potential (σ and ϵ values) with the diameter of the elements [62]. To obtain appropriate σ and ϵ values for the interaction of different elements, we employed the Lorentz-Berthelot mixing rules ($\epsilon_{12} = \sqrt{\epsilon_1 \times \epsilon_2}$ and $\sigma_{12} = (\sigma_1 + \sigma_2)/2$, *subscripts represent different elements*) [62].

As Fig. 1a shows, the scanned probe is formed by a single atom, which is connected to the base of the microscope with elastic springs and the interaction potential is calculated in three dimensions. As Fig. 1b demonstrates, the equilibrium point along z-direction for the normal force set point is found by equating the force acting on the tip along z-direction to energy stored on the spring (first equation in Fig. 1a). Surface corrugation is calculated by using the constant force profile. Systems of coupled differential equations, the second equation in Fig. 1a, are solved by using the ode45 function of MATLAB, while constraining the relative error to 10^{-10} [63]. Lateral forces acting on the tip is calculated by finding the force in the spring. To simulate the movement of the scanning force microscopy experiments, the tip starts with zero velocity at the left border of the scan area with relaxed springs. The transient part of the solution disappears within the first 5–6 Å for initial conditions and tip velocities (v_M) used in our calculations (250 nm/s ≤ v_M ≤ 2000 nm/s). We excluded the transient part of the solution in our statistical analyses. The energy dissipation due to friction is calculated with the dot product of lateral forces (Fig. 1c) and displacements (shown as an inset in Fig. 1c), which is equal to work done by lateral forces acting on the tip.

3. Results

We performed calculations with two-dimensional PT model to explore alloy composition, structure, normal load, and velocity dependence of frictional properties of bulk metallic glasses. Fig. 2a discloses a monotonic increase of surface corrugation with the number of alloy elements, surface disorder, and normal load. Fig. 2b displays the evolution of lateral forces acting on the tip as a function of normal load for different alloy compositions. Our calculations disclose that BMGs have three discrete friction regimes as a function of normal load. Fig. 2b reveals that lateral forces acting on the tip increases with the normal load; however, alloy composition does not have any major contribution for normal loads up to 2.8 nN (regime I). Unary crystal surface, unary glass surface, binary, and ternary BMG models have indistinguishable lateral forces in regime I. Between 2.8 nN and 4.1 nN (regime II) we observe a transition with variations in friction: unary crystal, binary, and ternary alloys have similar frictional forces, and unary glass structure exhibits the lowest frictional forces. For normal loads larger than 4.1 nN (regime III), friction is dominated by surface disorder and the rank of frictional forces are parallel to surface roughness presented in Fig. 2a. Besides, quarternary alloy compound exhibits the largest frictional forces and surface corrugation in all three regimes. The normal load dependence of frictional forces for quarternary alloy changes which is outlined with two different slopes (dashed lines in Fig. 2b) for regime I and regime II-III. Fig. 2c displays that energy dissipation due to friction for unary, binary, and ternary alloys increases parallel and has only saddle differences in regime I. The unary glass structure unveils smallest energy dissipation in regime II. Also, binary and ternary alloys dissipate more energy than unary systems with increasing loads in regime III. Quartenary alloy composition presents less than 10% more energy dissipation in regime I up to 2 nN normal loads and energy dissipation due to friction infliates for larger normal loads.

We also calculated the variation of lateral forces acting on the tip as a function of sliding velocity of the microscope body, alloy composition, and surface structure with two-dimensional PT model. As Fig. 3 summarizes, surface corrugation does not change with sliding velocity, which represents ideal experimental conditions. If the microscope tracks the surface with constant force mode and controller reacts fast enough to variations in topography, surface roughness does not change with velocity in experiments. Fig. 3b reveals that friction increases logarithmically with sliding velocity. Besides, there is no distinct dependence of friction on alloy composition and surface structure up to 1.3 μm/s scan velocities. Between 1.3 μm/s and 2 μm/s sliding velocities, the friction of unary glass structure is more than unary, binary, and ternary glass structures. Quarternary glass structure exhibits a larger frictional force for the entire range of velocities; however, it also