Wear 266 (2009) 1003–1012

Contents lists available at ScienceDirect

Wear

journal homepage: www.elsevier.com/locate/wear

Microstructural modeling of adaptive nanocomposite coatings for durability and wear

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ARTICLE INFO

Article history:
Received 22 May 2008
Received in revised form 17 December 2008
Accepted 10 February 2009
Available online 21 February 2009

Keywords:
Solid lubrication
Finite-element modeling
Sliding wear
Nanocomposite coating
Thin-film
Transfer film

ABSTRACT

Adaptive thin-film nanocomposite coatings comprised of crystalline ductile phases of gold and molybdenum disulfide, and brittle phases of diamond like carbon (DLC) and yttria stabilized zirconia (YSZ) have been investigated by specialized microstructurally based finite-element techniques. One of the major objectives is to determine optimal crystalline and amorphous compositions and behavior related to wear and durability over a wide range of thermo-mechanical conditions. The interrelated effects of microstructural characteristics such as grain shapes and sizes, local material behavior due to interfacial stresses and strains, varying amorphous and crystalline compositions, and transfer film adhesion on coating behavior have been studied. The computational predictions, consistent with experimental observations, indicate specific interfacial regions between DLC and ductile metal inclusions are critical regions of stress and strain accumulation that can be precursors to material failure and wear. It is shown by varying the composition, resulting in tradeoffs between lubrication, toughness, and strength, the effects of these critical stresses and strains can be controlled for desired behavior. A mechanistic model to account for experimentally observed transfer film adhesion modes was also developed, and based on these results, it was shown that transfer film bonding has a significant impact on stress and wear behavior.

1. Introduction

Computational modeling of thin-film coating wear has traditionally been based on the homogenization of coating properties to compute wear rates [1–5]. In contrast, nanocomposite thin-film (1 μm) coatings may comprise different material constituents, with each one being used for a desired behavior, such as lubrication, toughening, and strengthening [6]. For these advanced materials there is a need to understand how composition and microstructure [7–10], as well as velocity accommodation modes (VAMs) [11,12] affect the wear response and endurance. Hence, there is a need to (i) develop mechanical models to evaluate how coating microstructure and composition impact tribological properties as well as (ii) provide predictive capabilities to tailor multi-constituent thin-film response at the coating design stage.

Recent experiments [13] and processing have identified thin-film nanocomposite coatings with different combinations of crystalline and amorphous constituents exhibiting intrinsic low-friction that is adaptive in real time to changes in the environment as well as possessing good wear resistance and durability. These multicomponent coating systems provide good tribological performance over a greater operational range than a single phase coating can provide. From a design standpoint, these coatings combine the mechanical advantage of nanostructured hard phases such as nitrides and carbides with friction modifying phases. For example, the co-deposition of nanocrystalline TiN with either amorphous hydrogenated carbon (a-C:H) [14] or hydrogen free carbon (a-C) [15] results in enhanced hardness and good tribological behavior. More recently, nanocomposite coatings consisting of gold (Au), yttria stabilized zirconia (ZrO_2–Y_2O_3, YSZ), molybdenum disulfide (MoS_2) and DLC have been developed. These systems are referred to as adaptive coatings in that low wear, environmental stability, and low-friction coefficient can be attained in dry, humid, and high temperature (500 °C) operating conditions [16]. This coating performance is highly promising for a myriad of thermo-mechanical and wear applications.

If the mechanisms that result in improved wear and thermo-mechanical response can be accurately identified, then the constituent components and coating properties can be further optimized. Hardness improvements in nanocrystalline materials are understood to be controlled by resistance to dislocation formation and movement [17]. Toughness improvements can be achieved with the addition of ductile materials. Determining optimum configurations for multicomponent mixtures with lubricating

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doi:10.1016/j.wear.2009.02.004

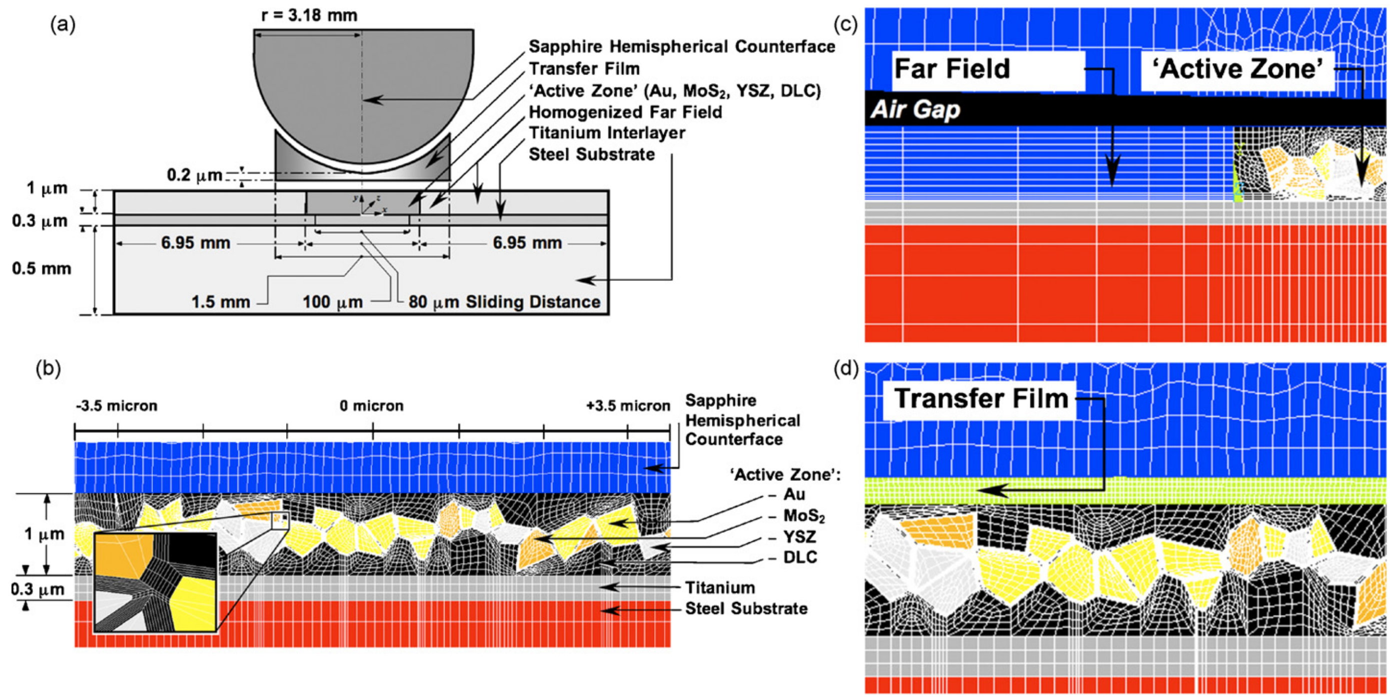

Fig. 1. (a) Dimensions and materials involved in the nanocomposite coating finite-element models. (b) The center of the 'active zone' underneath the slider. The zoom shows the level of detail in meshing of the DLC borders around each inclusion. (c) The transition between the active zone and the homogenized coating region. (d) The 'active zone' underneath the indenter with a transfer film of 200 nm thickness.

phases is challenging as optimizing hardness is not the only concern. What is not known or easily determined are what specific combinations of crystalline, amorphous, brittle, and ductile materials would be optimal, and what the dominant microstructural characteristics are that affect and control this adaptive behavior.

The major objective of the present study is to use microstructurally based finite-element techniques to examine how deformation and failure modes evolve in a simulated sliding contact of a multicomponent, nanostructured composite coating. In this study, detailed finite-element simulations of a linear reciprocating ball-on-flat configuration are used to examine local strain and stress evolution as a function of composition and scale. Single-component coatings of each constituent (Au, YSZ, MoS_2, DLC) were modeled and used as a limiting case to determine the effects of grain morphology, interfacial regions between the constituents, and mechanical properties for coatings with different compositions. Sliding simulations were undertaken to demonstrate the influence of tangential forces on plastic deformation, fracture, and transfer film formation. Transfer film (TF) models were also developed, and the TFs were represented as both a free (unstable) or bonded (stable) third body in the contact. Based on this, third body velocity accommodation modes relating to experimentally observed wear and interfacial sliding were identified. Finally, sliding simulations were undertaken to demonstrate the influence of tangential forces on plastic deformations. In the wake of the sliding body, the stress state is analyzed for potential Mode I fracture of the brittle DLC matrix material.

This paper is organized as follows: the finite-element modeling techniques are briefly outlined in Section 2. The effects of indentation stresses as a function of coating composition are presented in Section 3. Models of sliding and transfer films for adaptive multicomponent coatings are presented in Sections 4 and 5. In closure, general conclusions pertaining to optimal coating composition and the effect of transfer film bonding and sliding on the state of stress in the coating and the transfer film are presented.

2. Finite-element model and microstructural representation

A two-dimensional finite-element plane-strain model was used in the indentation and sliding simulations. Based on a convergence analysis, 125,000 quadrilateral elements were used for the simulations. The coating was represented as two regions: (1) a far-field region with elements of homogenized properties and no microstructural morphologies, and (2) an active zone centered beneath the slider (Fig. 1) with relevant microstructural morphologies, constituents, and sizes. This active zone is essentially a representative volume element (RVE) that accounts for physically realistic crystalline and amorphous microstructures. This level of morphological detail cannot be represented over the entire coating, since it would be computationally prohibitive due to the mesh size requirements associated with grain and inclusion sizes and shapes. More critically, by using this two-field approach, material behavior can be investigated at appropriate physical scales within the active zone. It should also be noted that the model system has significantly different physical scales [13]: coating thicknesses on the order of microns and grain sizes on an order of nanometers, and an indenter or slider on the order of millimeters. By using this two-field approach, interrelated material and system behavior at different physical scales can be accounted for.

The coatings were modeled based on the nanocomposite coating specimens prepared by Baker et al. [7] and the test geometry described by Chromik et al. [13]. The model is a representation of nanocomposite coatings on a 14×0.5 mm 440C steel coupon with a 0.3 μm thick uniform interlayer of pure titanium (for coating adhesion) between the steel substrate and the coating (Fig. 1(a) and (b)). Far-field regions away from the center of the steel substrate were assigned homogenized material properties based on reported experimental measurements [7,13].

The active microstructural zone, Fig. 1(a) and (b), is a 100-μm wide region at the center of contact. This region directly underneath the indenter is a physical representation of the coating constituents