Tribology International 103 (2016) 113–120

Contents lists available at ScienceDirect

Tribology International

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

Adhesion between ferrite iron–iron/cementite countersurfaces: A molecular dynamics study

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ARTICLE INFO

Article history:
Received 21 March 2016
Received in revised form
11 June 2016
Accepted 21 June 2016
Available online 22 June 2016

Keywords:
Molecular dynamics
Adhesion
Cementite
Iron
Commensurability

ABSTRACT

The adhesive properties of Fe(110)/Fe(110) and $Fe_3C(001)$/Fe(110) countersurfaces have been investigated by using classical molecular dynamics simulations. The simulation results show that Fe_3C/Fe exhibits a relatively lower adhesion compared to the Fe/Fe. Additionally, the temperature dependence of the adhesive properties between 300–700 K has been examined. The results demonstrate that, with increasing the temperature, the values of the adhesion force and the work of adhesion continuously decrease in the case of Fe_3C/Fe; they initially slightly increase up to 500 K then decrease in the case of Fe/Fe. Furthermore, the effect of lattice coherency between Fe/Fe has been examined and found to slightly reduce the adhesion. These results explain how carbides improve galling resistance of tool steel observed during dry sliding.

1. Introduction

In most cases, sliding between surfaces results in the progressive loss of material from the interacting surfaces, i.e. wear. Different types of mechanisms are defined, but the most general classification is abrasive scratching or adhesive mechanisms. Abrasive wear occurs due to cutting or ploughing of the softer surface by hard surface protrusions of the counter-surface or by hard third-body particles. Adhesive mechanisms occur at the atomic scale as bonds are formed between the surfaces, which in the absence of low shear-strength layers such as oxides for metals may possess strengths comparable to phase boundaries. In sheet metal forming, adhesive wear is of significant importance. During the forming process, metal surfaces are slid against each other under high contact pressures that results in wear of the sheet material, which is often referred to as galling. Galling is a multi-stage process where sheet material is continuously transferred to the tool surfaces by adhesive wear, which subsequently leads to abrasive scratching as the transferred material accumulates on the surface.

Tool galling resistance may be improved by optimization of the tool microstructure. Several publications [1–3], have shown that using tool steels with a high amount of primary second phase particle, i.e. carbides or nitrides, significantly improves the tool life. However, the underlying wear mechanisms are still unclear. In Refs. [2,4], the tool surface was studied in laboratory scale experiments of wear in sheet metal forming, including interrupted tests, to monitor the progression of tool damage. It was found that sheet material transfer initiated at the tool metal matrix and grew in size to form a continuous transfer layer covering the contact area. However, the amount of material transferred to ceramic primary particles was less than to the matrix. It was speculated that the mechanisms were due to lower adhesion between ceramic/metal interfaces as compared to metal/metal interfaces. The process of initiation and material transfer occurs at nanoscale scale level is inaccessible by experiments. Therefore, atomistic simulation becomes a vital tool to explore the interface structure and the adhesion between the metal surfaces at atomic level. In literature, a bunch of theoretical studies on adhesion between bcc metal/carbide-nitride are available. For example the results of ab initio calculations have shown a negative interface energy between bcc Fe/MN-MC (M=V, Nb and Ta), see Refs. [5–7]. Furthermore, Song and Sorolovitz [8], used molecular dynamics simulation to study the adhesive between asperity and metal flat surface, they showed that changing adhesion between surfaces can considerably reduce the material transfer volume by factor 1/2. In the present work, to further elucidate the influence of tool microstructure on adhesive wear, we investigate the factors that governing the adhesion between ferrite iron–iron/carbide interfaces such as temperature and commensurability by means of molecular dynamics simulation and the second-nearest neighbor modified embedded atom

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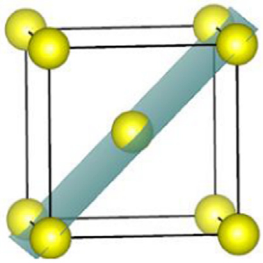
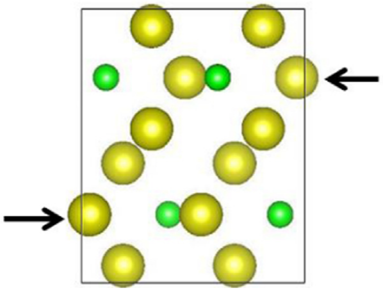
http://dx.doi.org/10.1016/j.triboint.2016.06.027
0301-679X/

Table 1
Unit cell of bcc-Fe and orthorhombic Fe_3C according to Fe–C potential. The yellow and green colors represent Fe and C atoms, respectively. The black arrow denotes the position of two of the four Fe atoms in their special positions in cementite.

	Body-centered cubic Iron	Orthorhombic Cementite (Fe_3C)
Unit cell		
Lattice constant (Å)	$a_0 = 2.8636$	$a = 5.16,\ b = 6.32,\ c = 4.66$

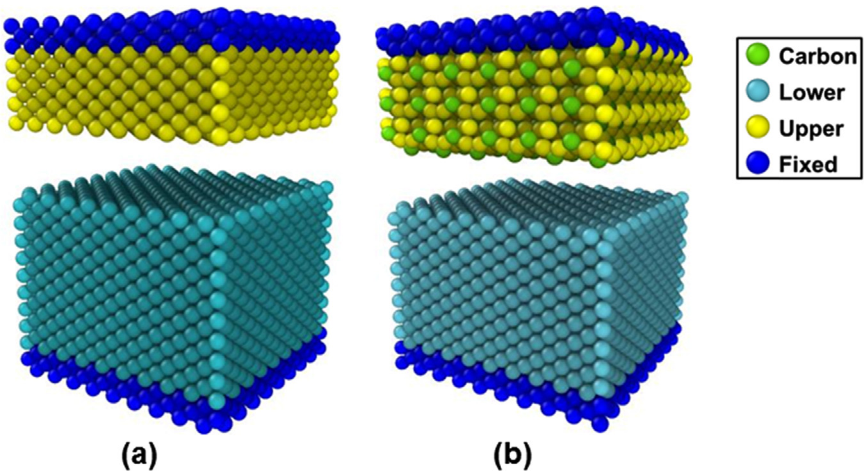


Fig. 1. Schematic showing MD model (a) Fe/Fe, and (b) Fe_3C/Fe configuration.

methods (2NN-MEAM) potential. We consider Fe_3C (cementite) as metastable prototype of carbide particles since it is commonly observed in low-alloy carbon steel [9].

2. Computational details

The MD sample was composed of two infinitely slabs aligned horizontally and separated by about 10 Å. In order to evaluate the chosen potential model and verify the results, we performed calculation for unrelaxed surface energy for both bcc-iron and orthorhombic Fe_3C. The results indicate that the (110) and (001) surface of bcc-iron and orthorhombic cementite, respectively, have the lowest surface energy. Hence, we decided to focus on these surfaces as they assumed to exhibit lower adhesion. In the case of Fe–Fe countersurfaces, the simulation cell composed of two, upper and lower, slabs in which the atoms are arranged in bcc-Fe lattice with (110) surface directed along Z direction. In the case of Fe_3C/Fe counterfaces the atoms in the upper block are arranged in orthorhombic-Fe_3C lattice with (001) surface. Furthermore, to reduce the effect of dimension misfit which arises due to lattice mismatch between Fe_3C and Fe, the number of unit cells in x and y

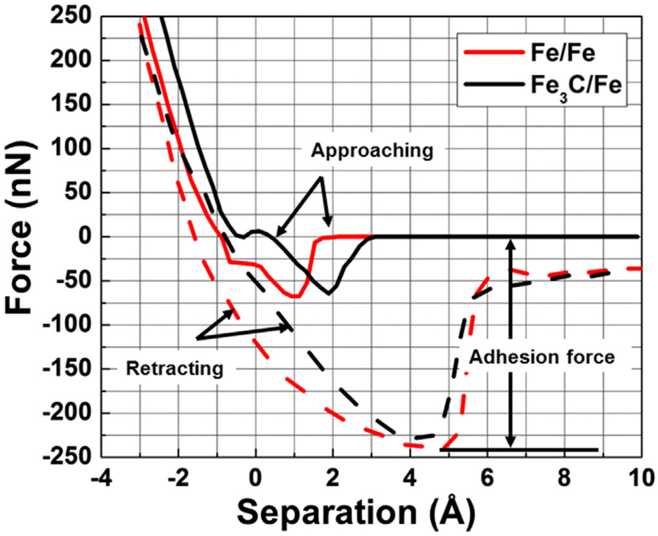


Fig. 2. Typical force-separation curves of Fe/Fe and Fe_3C/Fe countersurfaces at $T = 300$ K.