Tribology International 103 (2016) 432–439

Contents lists available at ScienceDirect

Tribology International

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

A computational study on the benefit of core-shell structured carbides to the erosion resistance of high-Cr cast irons

Juan Cui [a], Hong Guo [a,b], J.W. Li [b], D.Y. Li [a,*], Leo Parent [c], Harry Tian [d]

[a] Department of Chemical & materials Eng., University of Alberta, Edmonton, AB, Canada T6G 1H9
[b] School of Mechanical Eng., Taiyuan University of Sci. & Technol., Taiyuan, China
[c] Suncor Energy, Fort McMurray, AB, Canada T9H 3E3
[d] Metallurgical/Materials R&D, GIW Industries, Grovetown, GA 30813-2842, USA

ARTICLE INFO

Article history:
Received 4 May 2016
Received in revised form
1 August 2016
Accepted 2 August 2016
Available online 2 August 2016

Keywords:
High-Cr cast irons
Core-shell structure carbides
Model
Erosion

ABSTRACT

Hard M_7C_3 carbides in high Cr cast iron plays a crucial role in resisting wear. However, the hard carbides are less resistant to wear when impact force is involved, e.g., solid-particle erosion. Recent studies show that carbides may have a core (M_7C_3)-shell ($M_{23}C_6$) structure, leading to elevated erosion resistance. In order to maximize the beneficial effect, we conducted this computational study to investigate how the carbide configuration, including shell thickness, carbide shape and orientation, affects the erosion resistance. FEM was employed to analyze the stress distribution in the vicinity of carbide/matrix interface, which is crucial to interfacial failure and thus the erosion resistance. The information obtained from this study would be beneficial to optimization of the core-shell structured carbides.

1. Introduction

High Chromium Cast Irons (HCCIs) are widely used in mining, slurry pumping and manufacturing industries, where high resistance to erosion-corrosion and wear is require [1]. The excellent performance of HCCIs results from the combination of hard carbides (mainly M_7C_3 in hypereutectic HCCI) and ferrous matrix [2–4]. The matrix helps absorb impact force and enhance toughness of the material, while the hard carbides play a crucial role in withstanding the wearing stress [2,5]. In addition to the mechanical strength of the carbides, carbide/matrix interface also strongly influences the performance of HCCIs. In recent studies on HCCIs, it was noticed that under a certain fabrication condition, formed carbide showed a core (M_7C_3)-shell ($M_{23}C_6$) structure. The shell is softer than the core [6–11]. Such a core-shell structure has been experimentally demonstrated to be beneficial to the wear resistance of HCCIs, largely attributed to reduced stress concentration at carbide/matrix interface [7,8]. This helps improve the toughness of HCCIs through minimizing the risk of interfacial failure. The core-shell structured carbides are observed in HCCIs with high chromium contents [7,8]. Commercially used HCCIs have their chromium content in the range of 23–30 wt% Cr, in which the core-shell structured carbides may not form. However, in recent years, efforts have been made to push the Cr content to higher levels for more severe conditions involving large wearing stress and impact. In this case, high toughness is required [4]. Increasing the content of Cr, a strong carbide-forming element, helps increase hardness of HCCIs but this however deteriorates their fracture toughness. The formation of core-shell structured carbides makes it achievable to develop HCCIs with higher Cr contents while retaining desired toughness [8].

Tang et al. [7,8] investigated HCCIs with 45 wt% Cr, called 45-series, and demonstrated that HCCI 45-4 with 4 wt% C performed the best among the 45-series during abrasion and erosion tests. Core-shell structured carbides were observed in HCCI 45-4. Static stress analysis showed that the shell had its hardness between those of the harder core and soft ferrous matrix, which helped reduce the interfacial stress caused by the mismatch between the hard carbide and soft matrix [7].

In order to maximize the benefit of core-shell structured carbides in resisting wear, it is of importance to determine how the carbide configuration affects the wear resistance. Computational modeling is an effective approach for such investigation. Computational models proposed for wear simulation may be classified into two groups: macro-modeling and atomistic modeling. The former is proposed with existing tribological rules, empirical equations, assumptions or theories based on macro-mechanical properties [12], e.g., the removal of material is determined by the critical plastic strain. The continuum mechanical models or those with empirical rules can be used to determine the severity of wear under specific wearing conditions and to predict service life of a system with known material properties. However, the wear

* Corresponding author.
E-mail address: dongyang.li@ualberta.ca (D.Y. Li).

http://dx.doi.org/10.1016/j.triboint.2016.08.001
0301-679X/

resistance of a material is largely affected by its microstructure. The macro-modeling does not provide information for tribo-material modification through microstructure control. Thus, the macro-modeling is not used to predict material behavior but to determine the wearing condition for maintenance purpose, e.g., for estimating the service life of a pipeline subjected to erosion. Finite element method (FEM) is also used for wear simulation [13–15]. FEM analysis can provide information on the stress/strain distribution, which helps to predict the initiation of surface failure. However, continuous changes in surface geometry during wear make it difficult to simulate an entire wear process using FEM. Nevertheless, efforts are continuously made to facilitate wear analysis using FEM, e.g., Wang [18] combined FEM and a meshfree method to analyze erosive wear, which saved computing time. Atomistic modeling developed based on fundamental physics laws is effective for simulating wear of materials, such as the molecular dynamics simulation [16] and the first-principle technique [17]. The atomistic modeling help understand local wearing events and material behavior. However, the limited capability of current computing facilities makes it difficult to simulate wear of materials involving microstructural effects, which requires handling a large number of atoms.

In order to obtain more information on the effect of the core-shell structure on wear and maximize its benefits, a micro-scale dynamic method (MSDM) was employed to investigate how the shell thickness and orientation of the carbide would affect the erosion and impact resistance of the material. The MSDM is a simple and flexible technique, which has been proven effective for modeling different wear processes for materials design or modification [19–21]. The MSDM can be used to track the position and trajectory of material clusters during simulated wear processes based on Newton's law of motion and basic mechanical properties. MSDM has been successfully applied in modeling abrasive, sliding and corrosive wear processes [22,23]. In this study, stress/strain state of the core-shell structured carbide and its variations with the core-shell configuration were also analyzed with the finite element method (FEM) in order to better understand underlying mechanisms.

2. A core-shell structure HCCIs simulation model

2.1. MSDM model

2.1.1. The MSDM approach

The simulation study was conducted using a micro-scale dynamic method (MSDM), which has been described in previous publications [19–24]. For self-containing, a brief introduction to the method and main equations are provided here.

In this model, the erodent particle and the target material are discretized and mapped onto a 2D square lattices, respectively. Each lattice site represents a small volume of material. The strength of the bond between two sites is determined by mechanical properties of the materials involved, which can be measured experimentally. The movement of each lattice site is determined based on Newton's law of motion: $\vec{F} = m(d^2\vec{r}/dt^2)$, where $\vec{r}$ is the position vector of the lattice site and m is the mass of the site. The force exerted on this site, $\vec{F}$, includes the internal interaction force from adjacent sites and the external force from the erodent impact if the site is on the surface and have direct interact with the erodent. The site-site interaction force is proportional to the deformation of the bond between the adjacent sites, which can be expressed as: $\vec{f} = k\cdot\Delta\vec{l}$, where $\Delta l = l - l_0$ is the deformation of the bond between a pair of adjacent sites. l_0 is the length of bond in stress-free condition and l is length of bond with deformation. It should be noticed is that the term 'bond' here is not referred to the atomic bond between atoms but one similar to a spring connecting two adjacent material clusters or sites having a small volume, and $k = E\cdot l_0$ is the force coefficient or spring constant, which characterizes the interaction between two sites. When Δl is in the elastic region, E is the Young's modulus, $E = E_e = \sigma_y/\varepsilon_y$, where σ_y and ε_y are the yield stress and yield strain. Once Δl exceeds the elastic region, a so-called plastic modulus, $E = E_p = (\sigma_T - \sigma_y)/(\varepsilon_f - \varepsilon_y)$ is used, where σ_T and ε_f are the tensile stress and fracture strain. E_p reflects the resistance to irreversible plastic deformation and also the strain hardening capability. For the bond between metal sites, it has both elastic and plastic modulus, while for the bond between ceramic sites, it only has an elastic modulus. For a site on the target material surface, an external force $\vec{f}_p$ caused by particle impact needs to be taken into account. Thus, the total force exerted on a site denoted as p is expressed as:

$$\vec{F}_P = \sum_{q}^{n} k\cdot\Delta\vec{l}\,(p, q) + \vec{f}_p \tag{1}$$

where p and q represent two adjacent sites, n is the number of sites adjacent to site p; Then the velocity and the next position of site p after a time interval Δt may be determined by Newton's law of motion,

$$\vec{v}_{t+\Delta t}(p) = \vec{v}_t(p) + \frac{\vec{F}_p}{m}\cdot\Delta t \tag{2}$$

$$\vec{r}_{t+\Delta t}(p) = \vec{r}_t(p) + \frac{1}{2}\left[\vec{v}_t(p) + \vec{v}_{t+\Delta t}(p)\right]\cdot\Delta t \tag{3}$$

where $\vec{v}_t(p)$ and $\vec{v}_{t+\Delta t}(p)$ are velocities of site p at time t and $t + \Delta t$, respectively. m is the mass of site p; $\vec{r}_t(p)$ and $\vec{r}_{t+\Delta t}(p)$ are position vectors at time t and $t + \Delta t$, respectively. By repeating the calculations, trajectory and velocity of each site can be determined. A bond is not broken under compression but breaks if it is elongated with its deformation exceeding the corresponding fracture strain. A site or a cluster of sites is worn away during wear if all the bonds connecting to the site are broken. The volume loss is calculated based on the number of sites worn away according to the following equation:

$$\text{Volume loss} = \text{number of sites worn away} \times l_0^3 \tag{4}$$

More details have been described in previous publications [19–24].

2.1.2. The modeling procedure

For the MSDM modeling, Visual Studio 2010 professional (Microsoft) was used, and all components were written in C++. The microstructure of 45-4 HCCI consists of ferrite and carbides (single-phase carbide: M_7C_3; or core-shell structured carbide: M_7C_3 (core)-$M_{23}C_6$ (shell)). Fig. 1 illustrates a model system. Mechanical properties of various phases in the microstructure are given in Table 1 [7]. The target material was discretized and mapped on a lattice consisting of 6×3 units. Every unit contains 25×25 sites, as shown in Fig. 1. The carbide is designed as a hexagon according to SEM images reported [8,11,25]. The length of each bond (l_0) between a pair of adjacent site is 2×10^{-6} m, and time interval (Δt) was set as 8×10^{-11} s based on theoretical consideration for MSDM modeling [20]. For the carbide/matrix interfaces, both M_7C_3 and $M_{23}C_6$ are assumed to have similar chemical bonds or chemical interactions with the ferrous matrix. Thus, the difference in the overall carbide/matrix interfacial bond strength between M_7C_3 and $M_{23}C_6$ is mainly determined by the