Materials Science & Engineering A 669 (2016) 396–402

Contents lists available at ScienceDirect

Materials Science & Engineering A

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

Explore the electron work function as a promising indicative parameter for supplementary clues towards tailoring of wear-resistant materials

Jian Wang [a,b], Hao Lu [b], Bin Yu [b], Rongfeng Wang [a], Guomin Hua [b], Xianguo Yan [a], Leo Parent [c], Harry Tian [d], Reinaldo Chung [c], Dongyang Li [a,b,*]

[a] *School of Mechanical Engineering, Taiyuan University of Science and Technology, China*
[b] *Department of Chemical and Materials Engineering, University of Alberta, Canada*
[c] *Suncor Energy, Fort McMurray, Alberta, Canada T9H 3E3*
[d] *Metallurgical/Materials R&D, GIW Industries, Grovetown, GA 30813-2842, USA*

ARTICLE INFO

Article history:
Received 5 April 2016
Received in revised form
11 May 2016
Accepted 24 May 2016
Available online 25 May 2016

Keywords:
Electron work function
Hardness
Toughness
Wear resistance
High chromium cast iron

ABSTRACT

For materials used under dynamic loading conditions such as impact and impact wear, an appropriate balance between hardness and toughness is highly desired. However, determination of such a balance is challenging, since the toughness depends on both the mechanical strength and ductility, which complicates the judgement and control. Besides, local defects, poor phases and interfaces all could trigger local cracking and consequent global failure. These undesired structural or microstructural imperfections increase the difficulty in controlling the hardness-toughness balance. In this article, using high-Cr cast irons (HCCI) as example, we demonstrate that electron work function is a promising indicative parameter for supplementary clues to adjust the balance between hardness and toughness for HCCIs towards improved performance.

1. Introduction

Many materials used under dynamic loading conditions are required to possess both high hardness and high toughness. High-Cr cast irons (HCCIs) are such type of material, which are widely used as a wear-resistant material to resist abrasion and erosion in various industrial sectors, including mining, mineral processing, cement production, oil sand operation, and paper manufacturing, etc.[1,2]. The performance of HCCIs strongly depends on their microstructure, including the volume fraction, distribution and morphology of carbides [3,4] and properties of both the carbides and the ferrous matrix. HCCIs are generally hard with relatively low toughness. For wear under various wearing and loading conditions, both high hardness and toughness are desired [5] and they need to be appropriately balanced. Determination of such balance is challenging, since toughness depends on both mechanical strength and ductility. These two properties change in opposite directions when modified by, e.g., alloying elements and heat treatment. This complicates the judgement or determination of approaches for modifying HCCIs. Great efforts have been made to optimize HCCIs' microstructure by controlling carbide size and distribution in order to obtain high hardness while maintaining toughness at a satisfactory level [6,7]. However, microstructure control through alloying elements and heat treatment is largely based on trial-and-error tests without fundamentally sound guidelines.

Since HCCIs are generally hard, hardness is a less sensitive parameter used to guide HCCI design or modification [8]. For applications involving dynamic loading or impact such as solid-particle erosion at high velocities, more attention may need to be put on the fracture toughness. However, since toughness is a product of strength and ductility, and HCCIs' ductility is generally low, it is difficult to determine the optimal balance between hardness and toughness for maximized performance of HCCIs under various wearing conditions. Besides, local defects, undesired phases and interfaces could trigger local cracking and consequent global failure, which makes it more difficult to control the hardness-toughness balance. Thus, one has to perform a large number of trial-and-error tests, which is costly and time-consuming with limited effectiveness.

Mechanical properties of metallic materials are determined by their microstructure and properties of individual phases. The mechanical properties of individual phases are however fundamentally dependent on the electron behavior that governs the

---

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

http://dx.doi.org/10.1016/j.msea.2016.05.097
0921-5093/

atomic bond strength [9,10]. The electron behavior is largely reflected by electron work function (EWF or ϕ), which is the minimum energy required to extract electrons at Fermi level from inside a metal to its surface without kinetic energy [11,12]. A higher work function results from a more stable electron state, corresponding to a stronger electron-nucleus interaction or higher atomic bond strength, consequently leading to higher mechanical and electrochemical stabilities. Or in other words, metallic materials with higher EWFs are usually stronger and more resistant to electrochemical attacks. Although it is influenced by the surface state or condition, the work function fundamentally reflects the atomic interaction or atomic bond strength and is thus related to bulk properties [13,14]. The work function is proportional to $\rho_e^{1/6}$ (ρ_e is the valence electron density) [15]. A higher valence electron density corresponds to stronger electron-nucleus interaction or stronger metallic bonding. The metallic bond strength governs intrinsic mechanical properties. It has been demonstrated that EWF is closely related to many intrinsic material properties. For instance, the elastic modulus of metals shows a sixth-power relationship with work function [16,17]. Plastic deformation results in a rapid decrease in work function so that the work function can also be used to determine the initiation of plastic deformation and thus the yielding point [18]. The bonding strength of interfaces between phases can also be evaluated by interfacial work function [19]. A higher interfacial work function corresponds to a stronger interfacial bond. Furthermore, work function reflects the surface adhesion [20], thus affecting friction [21] and tribological processes [21–24], etc. The performance of materials appears to be related to the overall EWF to a certain degree, which is an integration of EWFs of individual microstructural constituents and microstructural features i.e. the morphology and spatial arrangement of the constituents. It is thus possible to obtain clues or supplementary information from the overall EWF, which helps better understand and guide tailoring materials.

In this study, we investigated hardness, toughness, electron work function (EWF), and resistances to sliding wear and solid-particle erosion for a number of HCCIs. Particular attention was paid to possible correlation between the work function and the properties of the HCCIs.

2. Experiment details

A set of HCCIs samples were fabricated using an induction furnace and compositions of the HCCIs are given in Table 1. The alloys contained 45%Cr and 4%C or 27%Cr and 2.5%C with other minor elements balanced by iron. The elements were selected based on the following reasons [25–27]:

- Chromium in the cast iron prevents formation of graphite and ensures the stability of carbide phases.
- Nickel and manganese are effective in suppressing the transformation of austenite matrix to pearlite and thus ensure a hard martensitic structure developing during cooling in mold.
- Silicon is added to improve the fluidity of the melt, which is of importance to the as-cast hardness.
- Molybdenum is a potent hardenability agent, inhibits formation of pearlite and forms Mo carbide.
- Vanadium is a strong carbide forming element.
- Boron is added to form hard borides and strengthen the ferrous matrix by solution-hardening.
- The addition of yttrium may improve the strength of cast irons and improve the passivation capability with formation of a more protective passive film.

Hardness of the samples was measured using a Mitutoyo hardness tester under a load of 5 N for 20 s. Each hardness value is an average of 10 measurements made at randomly selected locations on each sample. Toughness of the HCCIs was evaluated by Charpy impact tests. Each reported toughness value is an average of three measurements. Dimensions of samples for the impact test were 55 × 10 × 2 mm.

Sliding wear tests were performed on a pin-on-disc tribometer (CSEM Instruments, Neuchatel, Switzerland). The disc was the sample under study (15 mm × 8 mm × 5 mm) and the pin was a silicon nitride ball with its diameter equal to 6 mm. All tests were performed at a sliding speed of 2 cm/s along a circle path of 2.0 mm in diameter under a normal load of 10 N for 9000 rotations. Each wear test was repeated at least 3 times. Wear tracks and corresponding volume losses of the samples were determined using a confocal microscope (ZeGage 3D optical profilometer, Zygo Corp.).

Solid-particle erosion tests were carried out using a homemade air-jet erosion tester, which is schematically illustrated in Fig. 1. The erosion tests were performed at an impingement angle of 90° and a dry air flow was used to eject sand particles, generating a sand particle flow at a velocity of 55 m/s. The sand particle flow was delivered through a superalloy nozzle with its inner diameter equal to 4 mm. Each test consumed 2125 g fine sand (AFS 50–70) and the mass flow rate for the test was set as 177 g/min. The distance between the nozzle and sample surface was 10 mm. More details about the air-jet erosion apparatus can be found in a previous publication [28]. The purpose of using the high particle velocity and impingement angel of 90° was to perform the erosion tests under a condition in which the material toughness played a more important role in resisting erosion damage under larger impact forces. Weight losses of the samples caused by erosion were determined by weighing each sample before and after testing using a balance with an accuracy of 0.1 mg. The eroded scars were large and too deep for volume loss measurement using the optical profilometer. Thus, the weight loss was still used to evaluate the materials. Since the HCCIs have similar densities, the weight loss is meaningful for the erosion tests. Three erosion tests were performed for each HCCI and obtained results were averaged.

Table 1
Nominal composition of HCCIs under study and their impact energy values.

Sample	%Cr	%C	%Mn	%B	%Y	%Si	%V	%Ni	%Mo	Impact energy (J/cm^2)	Hardness
B0	45	4	0	0	0.5	0	0	0	0	2.1 ± 0.4	48.9 ± 1.5
B2	45	4	2	0	0.5	0	0	0	0	2.4 ± 0.5	52.0 ± 1.3
B5	45	4	1	0.5	0.5	0	0	0	0	2.0 ± 0.6	63.0 ± 0.6
B12	45	4	4	1	0.5	0	0	0	0	1.7 ± 0.3	64.1 ± 0.5
B16	45	4	4	1.5	0.5	0	0	0	0	1.5 ± 0.4	71.0 ± 0.7
B20	45	4	4	2	0.5	0	0	0	0	1.7 ± 0.2	63.0 ± 0.9
C1	27	2.5	0	0	0	0.8	0	0	0	2.5 ± 0.4	63.3 ± 0.5
C2	27	2.5	0	0	0	0	0	0.5	2	3.1 ± 0.5	63.0 ± 0.6
C3	27	2.5	1	2	0	0.5	6	1	2	2.3 ± 0.4	70.0 ± 0.1