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Potential application of electron work function in analyzing fracture toughness of materials

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ABSTRACT

Fracture toughness determines materials' resistance to fracture, which is measured often using impact or bending tests. However, it is difficult to evaluate fracture toughness of coatings and small samples. In this article, using white irons as sample materials, we explore a possible approach of using electron work function (EWF) as an indicator in evaluating fracture toughness of hard metallic materials. This parameter is promising for being utilized to analyze toughness of protective coatings and small objects as well as bulk materials. Through comparison with results obtained from impact tests and elastic modulus measurement, effectiveness of this EWF approach is demonstrated.

1. Introduction

Fracture toughness is one of important mechanical properties of materials, which is a measure of materials' resistance to facture. This property is crucial to materials which are required to have high reliability such as those used for components in aircrafts and space vehicles. Materials with higher fracture toughness are more reliable than those with low toughness. The fracture toughness of a material is usually evaluated using the stress intensity factor, K. When the stress intensity factor exceeds a critical value, K_c, facture occurs [1]. There are several standard methods for measuring the fracture toughness of bulk materials such as the impact and three-point bending methods [2]. However, the above-mentioned methods are not feasible for evaluating the fracture toughness of protective coatings, which is crucial to their performance [3,4]. Many protective coatings, e.g., wear-resistant ones, are generally hard and less tough. Indentation method can be used to evaluate fracture toughness of ceramic coatings by examining the configuration of generated cracks around the indent [5]. However, this method does not work for hard metallic coatings, e.g., those made of white irons or tool steels, since the coatings are hard but not as brittle as ceramic materials so that no cracking may occur around the indent. Thus, methods that can be used to evaluate the fracture toughness of protective coatings or films are highly desired.

In this article, we demonstrate that electron work function (EWF) is a promising parameter for evaluating the fracture toughness based on variations in EWF of the target material caused by repeated impact. EWF is the minimum energy required to extract electrons at Fermi level from inside a metal to its surface without kinetic energy [6]. Mechanical properties of materials are basically determined by the electron behavior that governs the atomic bond strength and ultimately the integrated mechanical properties [2]. Correlation between the electron behavior and mechanical properties of materials, including ductility and strength [7,8], has been theoretically studied using quantum mechanics and first-principles simulation. The quantum theories are however complicated and difficult to be feasibly applied in material characterization and design. Recent studies have shown that EWF is such a parameter which can be correlated to material properties in a straightforward manner, including Young's modulus, hardness, thermal expansion, and corrosion resistance [9–13]. Although EWF reflects the electron state at material surface, it fundamentally governs electron-nucleus interaction that determines the atomic bond strength and thus material strength [14,15]. It has also been shown that EWF is related to intrinsic ductility and brittleness [16], and is sensitive to surface morphology and cracks [17]. Thus, EWF could be

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Table 1
Fracture toughness, changes in Young's modulus and EWF of samples caused by repeated hammering.

	Fracture toughness (MPa m$^{1/2}$)	Changes in relative Young's modulus, $\frac{E_0-E_f}{E_0}$ (%)	Changes in work function, φ_0-φ_f (eV)	
			AFM	Kelvin probe
40−1	19.80	2.43	0.077	0.053
40−2	17.63	2.65	0.079	0.080
40−3	19.63	1.72	0.026	0.034
40−4	19.55	1.59	0.023	0.037
40−5	9.89	7.05	0.112	0.163
40−6	4.67	9.71	0.194	0.250

used to reflect fracture toughness of materials. In this study, using high-chromium cast irons with different carbon concentrations, we demonstrate that EWF is a promising indicative parameter for analyzing the fracture toughness.

When micro-cracks are generated in a hard and less tough material by impact, e.g., repeated hammering, structure integrity of the material deteriorates. This may result in a decrease in the electron density and thus lowered EWF [18]. Young's modulus of the material is also lowered due to loss of corresponding mechanical integrity or an increase of broken atomic bonds, which is proportional to the crack density [19,20]. A model is proposed to estimate the stability of cracks and fracture toughness of materials based on variations in Young's modulus [21]. Young's modulus is influenced by cracks, since the local effective stiffness may considerably decreases in the vicinity of a crack. Thus, both the fracture toughness and Young's modulus of a material decrease as the crack density increases. However, precisely measuring changes in Young's modulus of a coating on a substrate is challenging [22], although many studies on measuring surface Young's modulus using indentation techniques are reported in the literature [23,24]. Allowing for the fact that EWF is easy to be measured using Kelvin Probe on macro/micro-scales and using the multi-mode atomic force microscope (AFM) on nano-scale, EWF could be an alternative indicator for evaluating toughness for coatings and bulks as well.

In this study, using high-Cr cast irons as a sample material, we demonstrate the promise of evaluating fracture toughness based on EWF. Conventional impact tests and Young's modulus analysis were also carried out in order to verify the EWF analysis.

2. Experimental

Six high-Cr cast irons contain 40 wt% Cr and carbon concentrations ranging from 1 to 6 wt% were selected, which are denoted as samples from 40-1 to 40-6. SEM images of the alloys are illustrated in Fig. S1 in Supplementary data. It can be seen that samples 40-1 and 40-2 are in hypoeutectic states, 40-4, 40-5 and 40-6 are in hypereutectic states; and sample 40-3 is in a slightly hypereutectic state. The samples were repeated hammered for 2 min using a roto-hammer (Robert Bosch Tool Corporation, USA) at a frequency of 50 Hz. The head of the punching hammer, made of tool steel, had a semi-spherical shape of 5 mm in diameter. The impact energy of this punching machine was 2.207 N m. The process was well controlled in order to have the entire sample surface hammered homogeneously. Due to the low impact energy and short hammering process, little temperature rise at sample surface was detected, so that oxidation at sample surface was not a concern.

Young's modulus and EWF of the samples before and after the hammering were measured. Before EWF measurement, the samples were cleaned using an ultrasonic cleaner with reagent alcohol for 3 min to minimize the influence of contamination. EWFs of the samples were measured using a scanning Kelvin probe (KT Technology, UK) with a tip of 1 mm in tip radius. EWFs of the samples were further analyzed using a Bruker Multimode-8 AFM with the capability for local EWF mapping. Contact potential difference between the AFM probe (CoCr coated Si AFM probe with its nominal tip radius equal to 35 nm) and the sample was measured, which was then converted to EWF. Young's modulus of the samples was determined using a Resonant Frequency and Damping Analyser (RFDA) made by Integrated Material Control Engineering (IMCE, Belgium). During the measurement, an impulse was used to vibrate the sample and flexural vibration modes were analyzed, based on which Young's modulus was determined. Details about the Young's modulus measurement can be found in ASTM E1876 "Standard Test Method for Dynamic Young's Modulus, Shear Modulus, and Poisson's Ratio by Impulse Excitation of Vibration". The specimen for Young's modulus measurement had dimensions of 50 mm × 10 mm × 5 mm. Changes in sample dimensions by the repeated hammering process were very small and negligible.

Table 2
Roughness values of samples before and after repeated hammering.

Sample	Before repeated hammering (nm)	After repeated hammering (nm)
40−1	17.8	19.6
40−2	11.8	21.2
40−3	10.2	12.2
40−4	20.2	24.9
40−5	17.8	25.2
40−6	13.3	13.8

Fracture toughness of the samples was directly evaluated using conventional method based on ASTM E 399 standard (three-point bending test).

3. Results and discussion

Fracture toughness and changes in both EWF and Young's modulus caused by hammering are illustrated in Fig. 1 and the measured experimental values are listed in Table 1. As observed, the hypereutectic alloys 40-5 and 40-6 showed lower toughness, while hypoeutectic and eutectic samples with lower %C were tougher. The repeated hammering decreased both Young's modulus and EWF for all samples. The samples with lower fracture toughness showed larger decreases in Young's modulus and EWF.

The changes in EWF ($\Delta\varphi$) caused by repeated hammering were measured. As shown in Table 1, the average changes in EWF measured respectively using AFM and Kelvin probe show similar trends. Roughness values of the samples before and after the repeated hammering were determined using a confocal microscope. As illustrated in Table 2, the repeated hammering did not change much the roughness of the samples, suggesting that the minor changes in roughness should not be responsible for the variations in EWF caused by hammering. Sample 40-6 provides a good example. As shown, hammering resulted in little change in roughness of sample