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Elaborating the phases and mechanical properties of multiphase alloy: Experimental two-dimensional mapping combined with theoretical calculations

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ABSTRACT

The relationship between types of phases, microstructure and mechanical properties is always a critical challenge for the research and application of multiphase alloys. We report for the first time that NanoBlitz 3D method implemented in iNano is used to investigate the distribution of micro mechanical modulus and hardness for the entire complex multiphase alloy Fe-6.0W-5.0Mo-4.0Cr-2.0V-0.83C by constructing the two-dimensional mapping. In order to build the correlation between the microstructure and properties, the carbides in this tempering state steel are confirmed to be $Fe_3(W, Mo)_3C$, $Cr_{15.58}Fe_{7.42}C_6$ and V_8C_7 by acid etching and XRD refinement. The phases mapping is obtained by electron probe micro-analysis. Exact element ratio is characterized for the nano-scale multielement carbides precipitates. The Young's modulus and hardness of the precipitated carbides are up to 330 GPa and 22 GPa, respectively. The distribution range of Young's modulus and hardness is during 150 to 250 GPa and 2.5 to 7.0 GPa for the matrix phases, respectively. The experimental Young's modulus and hardness results are verified by first-principles calculations combined with Voigt-Reuss-Hill approximation. In fact, this work provides a successful demonstration to three-dimensionally characterize the micro mechanical properties for all the ceramics and alloys.

1. Introduction

Overall performances of the multiphase alloys are determined by the structure, properties and interaction of individual phases. The iron-based alloys with high tungsten and molybdenum content show high strengthen, hardness, sufficient fracture and wear resistance [1,2]. The essential properties are achieved by a microstructure consisting of a tough metallic matrix and a sufficient amount of a finely dispersed hard phase [3]. Collaboration of carbides and metal matrix plays an important role in the mechanical response of the steels, since carbides act as hard particles and dictate the wear resistance, and metal matrix guarantees the fracture toughness and bears the carbides. However, there is a lack of knowledge about the separate mechanical behavior of carbides and metallic matrix, mainly due to the experimental difficulties associated with its measurement. The previous research mainly focuses on the characterization of single point location on the single phase of the alloys by nanoindentation and electron probe micro-analysis [4,5]. Even though Casellas et al. performed the mechanical characterization of micrometer-sized carbides in tool steels, in terms of hardness, elastic modulus and fracture toughness [6], the distribution of the elastic modulus and hardness of the whole nano-scale carbides together with the matrix have never been reported so far. The phases mapping for the whole alloys is also seldom investigated in the literature. Moreover, the specific element ratio of the nano-scale carbides is hard to be confirmed just because of the dimensional restrictions [7].

In this work, we have reported for the first time, that the elastic modulus and hardness mapping of the entire microstructure for tempering state Fe-6.0 W-5.0Mo-4.0Cr-2.0V-0.83C (W6Mo2Cr4V2) steel by NanoBlitz 3D method. The results are verified by first-principles calculations. The composition mapping of all the phases in the steel are also characterized by the electron probe micro-analysis (EPMA). The aim of this work is to promote more accurate and comprehensive understanding on the correlation between microstructure and mechanical properties of the multiphase steel, and then control the properties through accurate microstructural design.

2. Experimental and Calculation Method

The studied object is selected as high tungsten and molybdenum steel at the tempering state, of which the phase composition and

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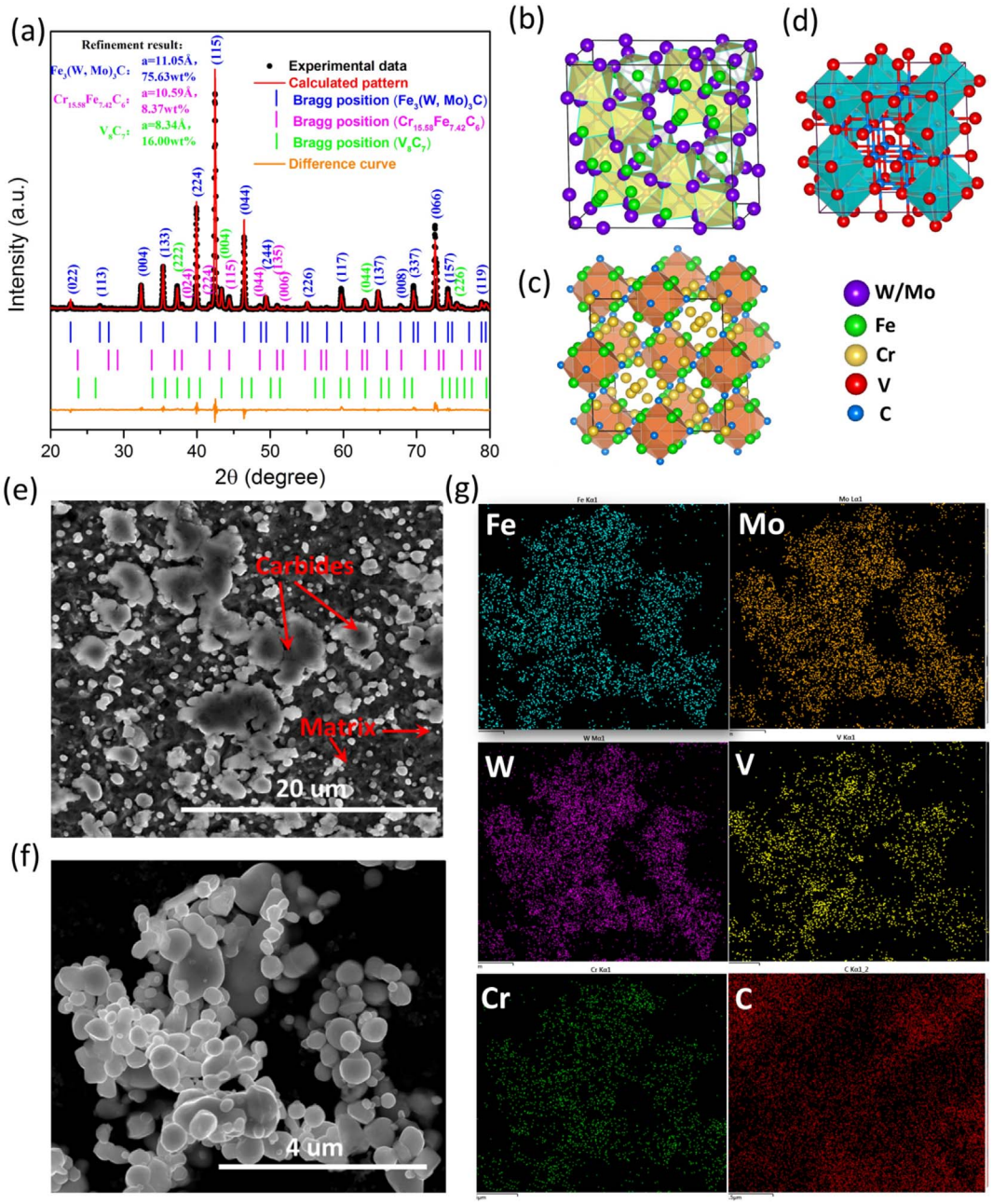

Fig. 1. Carbides types in W6Mo2Cr4V2 alloy. (a) X-ray diffraction analysis of the acid etching pure carbides; (b)–(d) crystal structures of Fe_3WMo_2C, $Cr_{15}Fe_8C_6$ and V_8C_7; (e) FESEM image of the microstructure of alloys; (f) FESEM image of the carbides powder; (g) EDS mapping results of the carbides powder.

distribution is close to the steel under service conditions. In order to characterize the structures and species of carbides without the influence of matrix, the massive alloy is deep etching in a 20% hydrochloric acid solution with heating under 80 °C for 2 h. Carbides powder is collected by filtering acid and ultrasonic cleaning of the residue in ethyl alcohol [8]. X-ray diffraction (XRD, Rigaku TTRIII) by Cu K_α radiation is used to characterize the species and crystal structures of the carbides powder. Microstructure of the alloy and the pure carbides powder are characterized by field emission scanning electron microscopy (FESEM, Quanta FEG 250). The phases' distribution mapping of the alloy and exact element ratio of the carbides particles are characterized by electron probe micro-analysis (EPMA, JXA-8530F). In order to reduce the height difference between carbides and metal matrix, the samples used to perform the nano-indentation are carefully prepared to obtain the flat surface by mechanical polishing, which can avoid large scatter and dispersion in nano-indentation behavior. The surface microtopography of the sample can be seen in Fig. S1. NanoBlitz three-dimensional (3D) release method implemented in the iNano instrument is used to perform an array of 30 × 30 indentations within a square area of 20 μm × 20 μm on the microstructure of this alloy. Distribution of the indentations can be seen in Fig. S2. The spacing between the indents is about 700 nm. Indentations are performed to a peak force of 1 mN at a rate of approximately 1 indent per second.

First-principles calculations based on the density functional theory (DFT) are implemented in Cambridge Serial Total Energy Package (CASTEP) code [9], with a plane-wave cutoff energy of 400 eV and a 4 × 4 × 4 Monkhorst–Pack k-point grid. Ultra-soft pseudo potentials (USPPs) are used to represent the interactions between ionic cores and valence electrons. The Broydene–Fletchere–Goldarbe–Shanno (BFGS) method is applied to optimize the crystal structure until the total energy changes are converged to 1×10^{-6} eV and the forces per atom are less than 0.02 eV/Å. In this work, generalized gradient approximation