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Stress induced phase transition on the medium-high carbon alloy steel hardfacing coating during the work hardening process: Experiments and first-principles calculation

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ABSTRACT

The stress induced phase transition on the medium-high carbon alloy steel hardfacing coating during the work hardening process was studied by experiments and first-principles calculation. The experimental results show that, the hardness of the specimens tempered for 2 h and 8 h at 480 °C before fatigue cycle are HRC 50.3 and HRC 50.1. The amounts of the retained austenite are 26.7 vt% and 7.3 vt%, respectively. With increase of the fatigue cycle, the amounts of the retained austenite in the tempered specimens decrease while their hardness increase constantly, until the amount of the retained austenite is decreased to 4.9 vt%. After fatigue cycle, the increments of the martensite grains with [001] and [101] orientations are much more than those with other orientations, which indicates that, during the work hardening process, the austenite grain transforms to the [001] and [101] oriented martensite grain preferentially. The calculated results show that, when pressure is 0 GPa, the face-centered cubic austenite supercell is stable, while the body-centered tetragonal martensite supercell is unstable. With increase of the pressure, the stabilities of the austenite and the martensite both increase gradually. When the pressure is larger than 18 GPa, the martensite is more stable than the austenite. For the austenite supercell, the stable limit pressure is 39 GPa. The critical pressure of the stress-induced phase transition is 36 GPa.

1. Introduction

Cold rolling back-up roll is the main workpiece manufactured by medium-high carbon alloy steel during steel rolling production [1]. After being used for a certain period of time, it usually fail due to the contact fatigue damage and excessive wear on the surface [2,3]. The failed cold rolling back-up roll can be remanufactured by hardfacing (harden-face-welding) method to restore their dimension, shape and obtain higher performance [4–6].

In order to reduce the residual stress, the remanufactured cold rolling back-up roll should be tempered for short time after hardfacing [7]. However, during the actual steel rolling production process, the hardness of the hardfacing coating on the remanufactured cold rolling back-up roll increases obviously after being used for a period of time, which means that the work hardening occurs [8]. The excessive high surface hardness of the cold rolling back-up roll will lead to deformation and cracking on the adjacent cold rolling roll, even causes the industrial accidents.

The work hardening behavior has been studied before. D.V. Wilson [9] calculated the work hardening reversible powers of the cubic crystal structure metals. Y. Estrin [10] described the plastic deformation and creep phenomenon in metal during the work hardening process by single-parameter model. B. Peeters [11] studied the work-hardening behavior of bcc polycrystals during changing strain paths. In recent years, with the advancement of the research method, the work hardening behavior has been investigated deeply. H. Idrissi [12] believed that the different work hardening rates between Fe-Mn-C steel and Fe-Mn-Si-Al steel under the same condition were caused by the internal immobile dislocations numbers. M. Koyama [13] considered that the work hardening behavior is mainly affected by twinning deformation and dispersion strengthened.

Although some progresses on the study of work hardening have been achieved, most researchers only focused their attention on the work hardening behavior itself or the stress concentration, which appears on the surface of workpiece. Up to now, the phase

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transition occurs during the work hardening process and the critical pressures of the stress-induced phase transition have been ignored.

Therefore, in this work, flux-cored wire for hardfacing the cold rolling back-up roll was developed to obtain the hardfacing coating specimens. Subsequently, the specimens were tempered at 480 °C for 2 h and 8 h respectively and the contact fatigue experiments were carried out. Then the mechanism of phase transition on the hardfacing coating of cold rolling back-up roll during the work hardening process was analyzed by hardness determination, microstructure observation and phase structure analysis. On this basis, the face-centered cubic (FCC) austenite supercell and the body-centered tetragonal (BCT) martensite supercell were established. Their cohesive energies and enthalpy differences at different pressures were calculated using a first-principles density functional plane-wave ultrasoft pseudopotential method, so the stress-induced martensitic phase transition during the work hardening process was analyzed from energetics, which can supply the theoretical basis for optimizing the microstructure of the hardfacing coating of cold rolling back-up roll and avoiding the work hardening behavior.

2. Experimental procedure

2.1. Experimental materials

The self-shielded flux-cored wire was manufactured, and the production process parameters are listed in Table 1. The outer shell of the flux-cored wire was made of low carton steel of H08A, and the core powders were composed of ferrosilicon, ferrochrome, ferromanganese and ferrotungsten.

2.2. Experimental methods

The matrix material was selected as cold rolling back-up roll steel plate, which was ground and cleaned with acetone before hardfacing. The bead-on-plate technique with flux cored arc welding (FCAW) was used to deposit the coatings via an automated system in which the welding torch was moved back and forth above the base metal at a constant speed in a multitrack overlapping process. The length of the single track was 100 mm, the coverage width was 8 mm, and the single layer thickness of the hardfacing coating was 2 mm. In order to avoid the effect of base metal on the microstructure and property of the hardfacing coating, each coating was welded for three layers. Subsequently, after the prepared hardfacing coating was air-cooled to ambient temperature, the specimens with the dimension of 10 mm × 10 mm × 15 mm were cut out by wire cut electric discharge machine. The hardfacing technology schematic diagram and the hardfacing coating specimen photograph are shown in Fig. 1. The chemical composition of the hardfacing coating is given in Table 2.

The hardfacing coating specimens were heated to 480 °C for 2 h and 8 h respectively before being cooled inside the furnace to room temperature. Then, they were carried out to fatigue cycle testing by JP-52 type fatigue testing machine. The schematic diagram for the fatigue cycle testing and the variation tendency for the contact force within one cycle are shown in Fig. 2, in which, the maximum contact force is 10 kN and the contact time in each cycle is 10 s. The fatigue cycles for the tempered samples were set to 200, 400, 600, 800, 1000, 1200, 1400, 1600, 1800 and 2000, respectively. Macro hardness of the specimens before and after fatigue cycle were measured using a HR-105A Rockwell hardness tester with a load of 150 kg for 10 s. The value presented is the average of the fifty measurements after the highest and lowest values are discarded.

Table 1
Production process parameters of the flux-cored wire.

Amount of coated flour	Powder dimension	Diameter of welding wire	Interface of welding wire	Width of steel band
46–48 wt%	40–60 mesh	Φ3.2 mm	O lap joint	12 mm

After metallographically polished, the tempered hardfacing coating specimens before and after fatigue cycle were corroded with 4% nitric acid alcohol. Subsequently, they were observed by a Hitachi S4800 field emission scanning electron microscope (FES-EM). The phase structures were analyzed by a D/max-2500/PC X-ray diffraction (XRD). The crystal structures of all phases were determined by a Jeolarm-200F transmission electron microscope (TEM). Moreover, the grain orientations were examined by Hitachi 3400 Electron Backscattered Diffraction microscope (EBSD).

2.3. Calculation methods

The 3D austenite supercell and martensite supercell models were established and their stabilities, total energies and enthalpy differences were calculated based on DFT (density functional theory) and employ the plane-wave pseudopotential total energy method as implemented in the VASP (Vienna ab initio simulation package) [14–16]. Projector augmented wave potentials [17] and the LDA (Local Density Approximation) of CAPZ (Ceperley-Alder-Perdew-Zunger) [18,19] were used for exchange correlation.

Unless otherwise specified, all structures were fully relaxed with respect to volume as well as all cell-internal atomic coordinates. The convergence of results with respect to energy cutoff Ec [20] and k-points number [21] was carefully considered, in which, Ec determines number of plane waves and k points does the sampling of the irreducible wedge of the Brillouin zone. In this work, Ec is set to 350 eV and the k point is set to 8 × 8 × 8, which make the convergence tolerance of energy of 1.0×10^{-5} eV/atom, maximum force of 0.03 eV/Å, and maximum displacement of 1.0×10^{-3} Å.

3. Experiment results

3.1. Hardness

Fig. 3 shows the hardness curves of the tempered specimens with different fatigue cycles. From it, the hardness of the specimen tempered for 2 h before fatigue cycle is HRC 50.3. With increase of the fatigue cycle, the hardness increases continuously and reaches HRC 56.5 when the number of fatigue cycle is 1200, which indicates that the work hardening occurs on hardfacing coating. With the further increase of the fatigue cycle, the hardness no longer changes anymore, remains HRC 56.5. For the specimen tempered for 8 h, its initial hardness is HRC 50.1. As the same as the specimen tempered for 2 h, the hardness of the specimen tempered for 8 h also increases with increase of the fatigue cycle. However, it reaches the maximum hardness HRC 51.9 only after 400 fatigue cycles, and then remains stable.

3.2. XRD

Fig. 4 shows the XRD curves of the tempered specimens after 0, 400, 1200 and 2000 fatigue cycles. From Fig. 4, the amount of the retained austenite in the specimens tempered for 2 h and 8 h both decrease with the increase of the fatigue cycle.

The amount of the retained austenite in steel can be calculated