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Effective design of new austenitic cast steels for ultra-high temperature automotive exhaust components through combined CALPHAD and experimental approaches

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ABSTRACT

Designing engines with higher power densities to comply with ever increasing emissions and fuel economy regulations requires the development of cost-effective alloys with superior properties than existing high-performance alloys. A new class of Nb-bearing austenitic heat-resistant cast steels showed promise to withstand exhaust gas temperatures of as high as 1000 °C. This paper describes the development of this new class of alloys using combined CALPHAD (CALculation of PHAse Diagrams) and experimental approaches to investigate the effect of C and N additions on the microstructure and tensile properties. Composition ranges were first established based on CALPHAD predictions to achieve the desired phases, and then four alloys of varying N/C ratios were cast and experimentally characterized to determine quantitatively the microstructure and mechanical properties. Microstructural characterization revealed that the NbC/Nb(C,N) phase transformed from "Chinese-script", a mixed flake-blocky morphology to faceted-blocky morphology as the N/C ratio increased. The area fractions of the different phases were quantified and agreed favorably with the calculated results. Alloys with the "Chinese-script" NbC/Nb(C,N) showed favorable tensile properties at room temperature and 1000 °C. Excessive δ-ferrite diminished the tensile resistance at 1000 °C, while limited quantity of (Cr, Fe)$_{23}$C$_6$ did not show adverse effects.

1. Introduction

Environmental protection and fuel economy regulations for automobiles and trucks are becoming more stringent around the world. To meet these regulations, manufacturers are pursuing many strategies and technologies to reduce emissions and improve fuel economy. One strategy is to increase the power density of the engines through the use of turbocharging, which can improve fuel economy without sacrificing vehicle performance [1,2]. However, moving to high power density engines increases the exhaust gas temperature with a commensurate increase in the operating temperature of components such as exhaust manifolds and turbocharger housings. Surface temperatures (skin temperatures) of the components in contact with the exhaust gas can reach to as high as 1000 °C, which is more than 200 °C higher than current operating temperatures [2,3]. These increased temperatures are above the operating ranges of the incumbent materials such as high-silicon, high-molybdenum ductile cast iron and ferritic cast steels. Existing high-performance alloys that are capable of operating at these temperatures are significantly more expensive than the incumbent materials [1]. Therefore, it is of great interest to develop a new class of alloys that can meet the high temperature performance requirements, but at a lower cost than the currently available alloys.

Nb-bearing austenitic stainless steels are attractive candidates because of their excellent corrosion resistance and mechanical properties at high temperatures [4]. These steels are widely used in chemical, nuclear and petroleum industries, and demonstrate promising creep resistance at temperatures near 800 °C [5,6]. For automotive exhaust components, cast steels with higher elevated temperature properties, including tensile and creep strength, thermal fatigue life, and oxidation resistance, are required for temperatures in excess of 1000 °C, while maintaining sufficient castability to cast complicated shapes [3,7]. Previous studies on wrought austenitic steels showed that Nb(C,N) precipitation had potential to improve the mechanical properties of these alloys at 1000 °C [6,8].

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Table 1
Measured chemical compositions of the experimental alloys (wt%).

Alloy	Fe	Cr	Ni	Si	Mn	Nb	S	P	C	N	N+C	N/C
4C0N	Bal.	18.42	9.16	0.49	0.86	2.00	0.007	0.013	0.40	0.01	0.41	0
3C2N	Bal.	19.68	10.12	0.80	0.93	2.09	0.008	0.013	0.29	0.15	0.44	0.52
2C2N	Bal.	20.91	9.60	0.86	0.95	2.16	0.008	0.014	0.21	0.22	0.43	1.05
2C4N	Bal.	21.32	9.88	0.92	0.95	2.18	0.007	0.014	0.23	0.36	0.59	1.57

To date, there has been limited research to investigate the effect of C and N additions on the as-cast microstructure and mechanical properties of Nb-bearing austenitic cast steels [4,9,10]. Therefore, the objective of this research is to investigate the effect of C and N on microstructure and tensile properties of Nb-bearing austenitic heat-resistant cast steels at room temperature and 1000 °C. The approach is to first design a series of experimental alloys with variations of C and N additions using a CALPHAD (CALculation of PHAse Diagrams) approach. This is complimented with microstructural characterizations and tensile tests at room temperature and 1000 °C. The relationship between composition, microstructure and tensile properties were evaluated, with emphasis on the role of C and N additions. The thermodynamic calculations were compared with the experimental results and if necessary will be used to make adjustments to the CALPHAD calculations to improve the fidelity of future predictions.

2. Design austenitic cast steels through Combined CALPHD and experimental approaches

The general concept for developing an austenitic cast steel with improved mechanical properties at high temperatures includes stabilizing the austenitic single-phase matrix, strengthening grain boundaries and interdendritic regions, and eliminating deleterious aging-induced phases (σ, Laves, etc.) [11,12]. The compositions of new alloys are designed to achieve these desired microstructures. Based on the economic considerations and temperature requirements, the 20Cr-10Ni type austenitic steel was selected for this study, instead of the 25Cr-20/30Ni (HK/HP type) steel which is more prevalently used at high temperatures [13,14]. Previous studies indicated that a relatively high Nb content of 2.0 wt%, was preferred for the experimental alloys compared to that of the commercially available austenitic cast steel (CF8C-Plus, 0.8 wt%) which is used at 850 °C [11,15,16]. In addition, Si (0.8 wt%) was added to improve the oxidation resistance at high temperature. Due to the relatively large additions of ferrite stabilizers (Cr, Nb and Si) and the strict control of Ni content, extra austenite stabilizers (Mn, C and N, etc.) are desired to aid in the stabilization of the austenitic matrix. Since both C and N are interstitial elements, powerful austenite stabilizers and Nb(C,N)-forming elements, they were presumed to significantly impact the as-cast microstructure and mechanical properties, in spite of their concentrations. Therefore, the compositional design in the current research would focus on the optimization of C and N additions in austenitic cast steels.

2.1. CALPHAD approaches

Multi-component phase diagrams of the Fe-20Cr-10Ni-0.8Si-1.0Mn-2.0 Nb-xC-yN (0≤ x≤0.6, 0≤ y≤0.5, wt%) alloy system were calculated using CALPHAD approach in the thermodynamic calculation software JMatPro™. Due to the complete diffusion of C and N during solidification, the thermodynamic equilibrium instead of the Scheil-Gulliver condition was calculated for a temperature range from 600 to 1600 °C at 1 °C intervals. The mass fractions of various phases (NbC/Nb(C,N), (Cr, Fe)$_{23}$C$_6$ and Cr$_2$(C,N)), which precipitate in solid phase transformation or induced aging, were calculated at a service temperature of 1000 °C as a function of C and N concentrations. The mass fraction of residual δ-ferrite was calculated at the predicted solidus temperature (1250 °C), and assumed that it was retained in the as-cast microstructure during solidification. The calculated fractions for each type of phases were collected and added to the isothermal diagrams at 1000 and 1250 °C.

2.2. Experimental approaches

2.2.1. Materials

Based on the thermodynamic calculations, four Nb-bearing austenitic cast steels with different N/C ratio (0–1.57) were selected and cast. The alloys were vacuum induction melted and cast into cylindrical ingots with a diameter of 80 mm and weighed approximately 20 kg each. The casting conditions were kept constant with a pouring temperature of 1550 °C, followed by furnace cooled to 600 °C, then air cooled to room temperature. The chemical compositions of the experimental alloys were quantitatively measured by NCS Testing Technology Co., Ltd. (NCS) and are listed in Table 1. The overall (C+N) content was constant (about 0.45 wt%), except for alloy 2C4N with an increased level (0.59 wt%).

2.2.2. Tensile tests

Tensile specimens were machined around the circumference of the ingot at a distance of 5 mm from the ingot surface. The tensile bars had a gauge length of 25 mm and cross-sectional diameter of 5 mm and were threaded dog-bone shaped. The tensile tests were performed at room temperature and 1000 °C. The 1000 °C specimens were heated in a three-zone furnace with a temperature control within 0.3 °C that was monitored using three thermocouples placed in the middle and both ends of the specimen. Extensometer with the resolution of 1 μm was directly attached to the specimen gauge length. The tensile tests for each experimental alloy were carried out using three samples at a strain rate of 10^{-3} s^{-1}.

2.2.3. Microstructural characterizations

Microstructural characterization on as-cast alloys was carried out using a ZEISS Axio Imager optical microscope (OM) and a ZEISS SUPRA 55 field emission-scanning electron microscope (FE-SEM) operated in secondary electron (SE) and backscattered electron (BSE) imaging modes. The grain structure was examined under a ZEISS AURIGA focused ion beam scanning electron microscope (FIB-SEM) operated in electron backscattered diffraction (EBSD) imaging mode. The average composition of the austenitic matrix and phases was quantitatively analyzed by a JEOL JXA-8530F field emission electron probe microanalyzer (FE-EPMA) equipped with five wavelength dispersive spectrometers (WDS). The diffraction crystals of LDE6H and LDE1H were specially integrated into this WDS system to exactly measure the C and N concentrations. The crystal structure of different phases was identified using a Rigaku X-ray Diffractometer (XRD) and a FEI Tecnai G2 F20 transmission electron microscope (TEM).

Metallographic specimens for OM and SEM observation were prepared by grinding with SiC papers up to 5000 grit followed by polishing using 0.1 μm diamond powder, and then electro-etching with an electrolyte of 7% HNO_3, 21% HCl, 21% H_2O and 51% CH_3OH for 5–20 s at 2 V. EBSD specimens were prepared using standard grinding and polishing techniques to a final vibratory polishing using a solution of 90% colloidal silica (0.02 μm) and 10% $NH_3 \cdot H_2O$. EPMA specimens