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Effect of lanthanum on the precipitation and dissolution of NbC in microalloyed steels

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ABSTRACT

The effect of lanthanum on the precipitation and dissolution of NbC in microalloyed steel was investigated using a combination method of thermo-mechanical experiment and the first-principle calculations. The interaction of niobium with lanthanum is attractive in the 2nn to 6nn shell, and that of carbon with lanthanum is relatively strongly attractive in 4nn(B) and 5nn coordination shells. These attractive interactions lead to an increase in the Nb and C solubility in fcc Fe, and a decrease in the chemical potential of these two solutes, thereby suppressing the formation of NbC. The strain-induced precipitation intensity was characterized using field emission scanning electron microscope (FE-SEM) and inductively coupled plasma optical emission spectrometry (ICP-OES). The experimental results reveal that after deformation NbC precipitated more in La free steel than in La addition steel. And since the relatively higher dissolution rate of NbC in La addition steel, the Zener pinning effect decreased slightly faster, leading to a higher coarsening rate of austenite grain during isothermally heating at 1200 °C.

1. Introduction

It is well known that hot rolled microalloyed steels can be strengthened by a combination of grain refinement and precipitation strengthening, using microalloying elements niobium, titanium and vanadium, individually or in combination [1–3]. During thermo-mechanical controlled processes (TMCP), the recrystallization process largely governs the final grain size of the micro-alloyed steels. One can obtain a fine grain size by maximizing the recrystallization nucleation rate and minimizing the growth rate of recrystallization grain. In this process, the driving force for recrystallization is stored strain energy, and the migration velocity of austenite grain boundary can be affected by two mechanisms: Zener pinning of the precipitates and drag effect of the solute [4–6]. The addition of Nb has been demonstrated to be an effective alloying element to control the recrystallization process in both pinning and drag ways. In addition, microalloying elements, such as titanium, vanadium, nitrogen and molybdenum, have frequently been added into steels to enhance the control of the Nb precipitation process, and thus the recrystallization [7–9].

In the past years, the addition of rare earth (RE) elements has been regarded promising in microalloyed steels [10–12]. Many studies have been carried out to investigate the effect of RE in steels [13–19], such as the purification, solidification, high-temperature oxidation resistance, corrosion resistance and phase transformation. Despite the progress in RE research so far, it still lacks systematical investigation into the effect of RE on the Nb precipitation and consequently the recrystallization during thermal processing.

In this work, to elucidate the effect of RE on the precipitation and dissolution behavior of NbC during thermo-mechanical process, two types of Nb bearing steels (La alloyed and La free) were selected for comparative reasons. The evolution of the precipitates with respect to the thermal heat treatment following the deformation was analyzed, and the fundamental mechanism of La effect on the NbC precipitation and dissolution kinetics was investigated using the fist-principle calculations, and subsequently the interactions between precipitates and recrystallization were clarified.

2. Experimental and computational approach

2.1. Experimental procedure

The materials used in this work consisted of two Nb contained microalloyed steels, the chemical composition of these two alloys are listed in Table 1. The first alloy, without addition of La, represents a reference Nb bearing microalloyed steel. The second alloy was designed to study the effect of La addition. The experimental steels were

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Table 1
Chemical composition of the experimental steels (wt%).

Steel	C	Si	Mn	P	S	N	Nb	Ti	La
P1	0.043	0.247	1.83	0.007	0.005	0.0027	0.085	0.012	0
P2	0.042	0.243	1.86	0.008	0.006	0.0027	0.087	0.013	0.0048

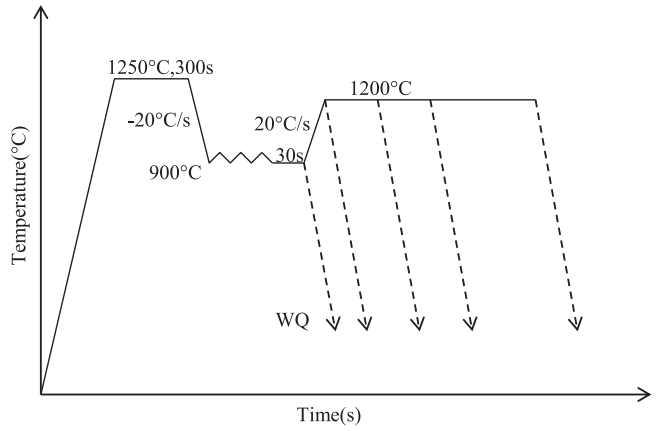

Fig. 1. Illustration of thermo-mechanical processing.

prepared by vacuum induction melting and cast into ingots. The ingots were homogenized at 1573 K for 2 h, and then hot rolled from 30 mm to 18 mm thickness.

For the case of NbC precipitation and dissolution, the hot deformation simulations were performed using a Gleeble-1500D thermo-mechanical simulator. The test specimens of 6 mm diameter and 15 mm length were machined from the hot rolled plates with the long axis parallel to the normal direction of the plate. As shown in Fig. 1, the specimens were reheated to 1250 °C for 5 min, and then cooled to the deformation temperature of 900 °C (this temperature is below the non-recrystallization temperature [20]) at a cooling rate of 20 °C/s, followed by a single deformation pass with a strain of 0.3 and a strain rate of 10/s. After isothermal holding for 30 s, the samples were reheated at a rate of 20 °C/s to a temperature of 1200 °C, and held for various times, subsequently water quenched to room temperature. For the microscopy examination, transverse specimens were machined from the quenched samples. The picric acid etchant was used to reveal the prior austenite grain boundaries. The average size of austenite grain was measured through the linear intercept method (ASTM E-112) using optical microscopy. The microstructure was characterized by the field emission scanning electron microscope (FE-SEM, ZEISS Supra 55) equipped with a nanometer probe energy dispersive spectrometer eter (EDS). The amount of Nb precipitated was measured by the inductively coupled plasma optical emission spectrometry (ICP-OES).

2.2. First principles methodology

To understand the effect of La on the precipitation of NbC, the interactions of La-Nb and La-C were investigated using the first-principles calculations. The first-principles calculations presented here were performed with DFT as implemented in Vienna Ab Initio Simulation Package (VASP) with the projector augmented wave (PAW) method and the generalized gradient approximation of Perdew-Burke-Ernzerhof functional (GGA-PBE) [21]. All calculations were performed in spin polarized. The computations performed within a 4×4×4 supercell including 256 atoms. The binding, energies were calculated with 350 eV plane-wave cutoff and 5×5×5 k-point meshes. The residual atomic forces in the relaxed configurations were lower than 0.01 eV/Å. After full structure relaxation, the calculated lattice parameter of fcc Fe is 3.52 Å, which is in good agreement with the experimental result (3.56 Å) [22]. The following calculations are based on this lattice constant and do not take into account the effect of temperature.

The binding energy of two defects is calculated as follows:

$$E_b = E_{tot}^{X,Y} + E_{tot}^{bulk} - E_{tot}^{X} - E_{tot}^{Y} \quad (1)$$

where $E_{tot}^{X,Y}$ is the total energy of the supercell containing a defect X-Y pair, E_{tot}^{bulk} denotes the energy of the supercell containing no defects, E_{tot}^{X} and E_{tot}^{Y} are the total energies of the supercell with a solute atom X or Y. A positive sign of the binding energy corresponds to the repulsive interaction between the two solutes.

Based on the calculated binding energy, the probability that a Nb (or C) atom locate at a site of a certain distance from La atom, i.e. the fractions of Nb (or C) at different nearest neighbor shells of La atom, can be calculated as follows [23]:

$$f_i = f_\infty \exp\left(\frac{-E_{b(i)}}{k_B T}\right) \quad (2)$$

where the subscript i represents a particular nearest neighbor shell, k_B and T denote the Boltzmann constant and the absolute temperature, respectively. f_∞ represents the fraction of sites filled with Nb (or C) atoms beyond the maximum interaction distance of La-Nb (La-C), i.e. the La-Nb (La-C) binding energy approaches zero, and can be expressed by:

$$f_\infty = \frac{C_C\,(or\ \ C_{Nb})}{1 + C_{La}\sum_{i=1,\,\max}\left(n_i \exp\left(\frac{-E_{b(i)}}{k_B T}\right)\right) - C_{La}\sum_{i=1,\,\max} n_i} \quad (3)$$

where C_C, C_{Nb} and C_{La} denote the concentration of C, Nb and La, respectively, n_i is the numbers of equivalent site in the ith nearest neighbor shell of La atom.

3. Result and discussion

3.1. Microstructure

After the solution treatment at 1250 °C for 5 min, the prior austenite grain sizes of these two steels were 57.56 μm and 62.91 μm, relatively, as shown in Fig. 2. For the specimens subjected to further compression at 900 °C followed by reheating to 1200 °C and holding for 100 s, the average grain size of the reference alloy was 59.9 μm, while that of the La addition alloy was 76.9 μm. The grain sizes of these two alloys increased by 4.1% and 22.2%, respectively. The austenite grain size may be affected by the NbC precipitate state [24]. The difference between the coarsening processes of these two steels indicates that the grain growth of the reference Nb bearing steel was inhibited in a greater degree by the small amount of precipitates, i.e. more precipitates dissolved into the matrix in the La addition steel during isothermal holding.

3.2. Precipitation and dissolution

During the deformation process, the evolution of the dislocation density ρ as the function of strain ε can be expressed as following [25]:

$$\frac{d\rho}{M \cdot d\varepsilon} = \frac{1}{\lambda \cdot b} - f \cdot \rho \quad (4)$$

where M denotes the Taylor factor (M=3.1 in austenite), b represents the Burgers' vector, f is a fitting parameter, and λ denotes the mean free path of the dislocation movement, which correlates to the grain size d_g and the distance between two precipitates d_{pre} [26]:

$$\frac{1}{\lambda} = \frac{1}{d_g} + k\sqrt{\rho} + \frac{1}{d_{pre}} \quad (5)$$

Therefore, the strain-induced precipitates will impede the disloca-