

Quantitative analyses of ferrite lattice parameter and solute Nb content in low carbon microalloyed steels

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Abstract

The effect of solute Nb on the ferrite lattice parameter in low carbon steels was examined using X-ray diffraction and related to atomic size difference. The concentration of solute Nb in ferrite of a furnace-cooled steel was successfully predicted using the measured coefficient of Nb atoms on the ferrite lattice parameter.

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1. Introduction

The carbo-nitride-forming elements such as Nb, Ti and V have great influence on microstructure and mechanical properties of low carbon microalloyed steels. A small addition of Nb to low carbon steels is very effective in grain refinement and precipitation hardening as solute Nb atoms or NbC precipitates. The amounts of the solute Nb and NbC precipitates in microalloyed steels have been investigated by using different experimental methods such as inductively coupled plasma atomic emission spectrometry (ICP-AES), transmission electron microscopy (TEM), and stress relaxation [1–4].

Although the size and chemical composition of the precipitates can be evaluated from TEM-EDS work, it is still difficult to acquire the amount of the precipitates, especially in the case of very fine particles less than 100 nm in diameter using TEM, ICP-AES, and mechanical tests.

The X-ray diffraction technique is expected to be useful to quantitatively determine the amount of the solute

Nb based on the relationship between the lattice parameters of austenite and ferrite and the concentration of an alloying element as follows [5–7]:

$$a_{\gamma}(\text{nm}) = 0.35770 + 0.00065 \times C + 0.00010 \times \text{Mn} \\ - 0.00002 \times \text{Ni} + 0.00006 \times \text{Cr} \\ + 0.00056 \times \text{N} + 0.00028 \times \text{Al} \\ - 0.00004 \times \text{Co} + 0.00014 \times \text{Cu} \\ + 0.00053 \times \text{Mo} + 0.00079 \times \text{Nb} \\ + 0.00032 \times \text{Ti} + 0.00017 \times \text{V} + 0.00057 \times \text{W} \quad (1)$$

$$a_{\alpha}(\text{nm}) = 0.28664 + 0.00006 \times \text{Mn} - 0.00003 \times \text{Si} \\ - 0.00007 \times \text{Ni} + 0.00005 \times \text{Cr} \\ - 0.00010 \times \text{P} - 0.00031 \times \text{Ti} + 0.00027 \\ \times \text{Ru} + 0.00035 \times \text{Rh} + 0.00029 \times \text{Re} \\ + 0.00037 \times \text{Ir} + 0.00049 \times \text{Pt} \quad (2)$$

where a_{γ} and a_{α} are the lattice parameters of austenite and ferrite, respectively, and the concentration of each element is in atomic percent.

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Eq. (1) includes the effect of Nb on the lattice parameter of austenite and the coefficient of Nb is 0.00079 nm per atomic percent. However, there are few articles about the effect of Nb on the lattice parameter of ferrite. The purpose of this study is to quantitatively investigate the coefficient of Nb on the lattice parameter of ferrite to evaluate the amount of the solute Nb in low carbon microalloyed steels.

2. Experimental procedure

The five ingots of Fe–X%C–0.2%Si–1.2%Mn–Y%Nb steels were prepared using a vacuum induction furnace. The chemical composition of homogenized ingots is listed in Table 1. The ingots were hot-rolled to 10 mm thick plates, from which the specimens of $15 \times 15 \times 2 \text{ mm}^3$ were machined, solution-treated at 1170 °C for 10 min in a vacuum furnace to fully dissolve Nb particles, which might form during hot rolling, and then furnace-cooled down to the room temperature. The samples were mechanically polished by using Emery papers of different grit sizes and the cloth pasted with alumina powders of about 1 μm . Finally, the samples were chemically polished using a chemical mixture of acetic acid 90% and perchloric acid 10%.

To examine the lattice parameter of ferrite, X-ray diffraction (XRD) tests were performed at room temperature after the calibration of the standard Si powders using “Rigaku D/Max-RC” diffractometer with the Cu target whose $K\alpha$ wavelength λ is 1.540562 Å. The scanning angle 2θ was between 35° and 140° and the step size was 0.01°. The lattice parameters were first calculated by applying the Nelson–Riley function [8] to each peak having different diffraction angles (2θ), and then final lattice parameter of the ferrite was determined by fitting the different lattice parameters obtained at each peak by using the least square method, and was listed with an error range in Table 1.

3. Results and discussion

3.1. Effect of Nb on ferrite lattice parameter

The effect of Nb on the lattice parameter of ferrite in the ultra-low carbon microalloyed steels (A1, A2, A3, A4

in Table 1) was examined by X-ray diffraction tests. Because the carbon content of the steels (0.003 wt.%) is too low to form NbC precipitates during furnace cooling, all Nb atoms can be assumed to remain as solutes in ferrite matrix.

Strictly speaking, however, the distribution of the solute Nb atoms would be unlikely uniform in the ferrite matrix during furnace cooling, because the segregation of Nb atoms to the grain boundaries can occur at such a slow cooling rate [9]. Nevertheless, the lattice parameters of polycrystalline materials have been widely measured as a function of the average solute content by using X-ray diffraction [10–12].

The variation in lattice parameter of ferrite is plotted against Nb content in atomic percent in Fig. 1. The lattice parameter of ferrite is almost linearly proportional to the Nb concentration and the slope ($k_{\text{Nb}} = 0.000625 \text{ (nm/at.\%)}$) is the coefficient of Nb on the lattice parameter of ferrite.

The intersection point between a fitted straight line and y-axis indicates the lattice parameter of ferrite without Nb atoms (0.286768 nm), which can also be calculated using Eq. (2) containing the coefficients of alloying elements such as C, Mn and Si on the lattice parameter of ferrite. The calculated lattice parameter of ferrite without Nb atoms (0.286707 nm) is in a good agreement with the experimental one of 0.286767 nm. The lattice parameter of ferrite of pure iron is taken as 0.28664 nm at 25 °C (JCPDS, Card 6-0696).

3.2. Effect of the difference in atomic radius between Fe and an alloying element on lattice parameters

Assuming that the variation in lattice parameters of austenite and ferrite with the addition of an alloying element is closely related to the difference in atomic radius [13] between Fe and the alloying element, the coefficients of alloying elements on the austenite lattice parameter in Eq. (1) are plotted against the difference in atomic radius between Fe and alloying elements in Fig. 2.

The coefficient of the alloying element on the lattice parameter of austenite is increased with the increase in difference in atomic radius between Fe and the alloying element. Specially, the coefficient of Nb in Eq. (1) does not seem different from that of Nb calculated using a fitted curve in Fig. 2.

Table 1
Chemical composition and ferrite lattice parameters of the experimental steels (wt.%)

Steel	C	Si	Mn	Nb	N	a_{α} (nm)
A1	0.003	0.20	1.21	–	0.0035	0.286767 ± 0.0000073
A2	0.003	0.20	1.21	0.020	0.0037	0.286778 ± 0.0000048
A3	0.003	0.20	1.21	0.050	0.0041	0.286786 ± 0.0000039
A4	0.003	0.20	1.20	0.080	0.0036	0.286797 ± 0.0000041
A5	0.040	0.20	1.22	0.082	0.0045	0.286788 ± 0.0000021

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