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Relationship between Crystal Structure of Inclusions and Formation of Acicular Ferrites

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Abstract: The formation mechanism of intragranular ferrites with acicular morphology was discussed. The ferrites were characterized by scanning electron microscopy. The results showed that the ferrites had an acicular structure with radial, symmetrical, and acicular laths, and that the inclusions were the nucleation sites of the intragranular acicular ferrites. Transmission electron microscopy (TEM) was used to characterize the inclusions. The results of TEM with energy dispersive spectroscopy and TEM-selected area electron diffraction indicated that the complex inclusions consisted of Ti-Al complex oxides and MnS. The jagged edges of the complex inclusions can be ascribed to the effects of the crystal structure. The stabilization energy U of the coordination polyhedron growth units varies with the type of connection according to the calculation results. A larger U corresponds to more stable growth units, which induces the preferentially oriented growth of inclusions, at which point acicular ferrites are formed.

Key words: crystal growth; crystal structure; acicular ferrite; inclusion; microstructure

The formation of fine intragranular acicular ferrites (IGFs) is an effective way of refining microstructure, resulting in an improvement in strength and toughness[1-4]. Medina et al. [5] revealed that the intragranular nucleation of acicular ferrites on inclusions led to a significant decrease in grain size to nearly 50%. The principal role of inclusions is to provide an inert surface for the heterogeneous nucleation of acicular ferrite laths[6]. Extensive researches have been carried out on the crystallographic orientation relationship between inclusions and ferrites[7-9]. Jin et al. [10] demonstrated that one or more ferrite grains nucleate from a single TiN particle but all ferrite grains have a Baker-Nutting (B-N) orientation relationship with the TiN particle. The observed B-N relationship between the intragranular ferrite grains and the TiN particles suggests that the intragranular nucleation of ferrites from these complex inclusions is promoted by the crystallographic coherency of TiN with the ferrites. However, few studies have focused on the crystal structure relationship between inclusions and intragranular acicular ferrites.

The relationship between crystal structure and growth units has been studied[11-13]. Based on the theoretical model of coordination polyhedron growth units, Zhong and Hua[14] demonstrated the relationship between the crystal morphology and the orientation of anionic coordination polyhedra in isomer (rutile, brookite, and anatase) and allomer (corundum, hematite, and ilmenite) crystals. The crystal habits of these crystals were found to be related to

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the stability of the anionic coordination polyhedron growth units. In trimorphs of TiO_2 (rutile, brookite, and anatase), the octahedral $[Ti\text{-}O_6]^{8-}$ is considered to be the growth unit. Since the crystallographic orientation of this growth unit is different in each of the trimorph crystals, the crystals show different morphologies. In corundum (Al_2O_3), hematite (Fe_2O_3), and ilmenite ($FeTiO_3$), the anionic coordination polyhedra are $[Al\text{-}O_6]^{8-}$, $[Fe\text{-}O_6]^{8-}$, and $[Ti\text{-}O_6]^{8-}$, respectively. These growth units have the same orientation and combination manner; therefore, the allomer crystals have very similar morphologies[15].

Despite what has been achieved so far, there is a need for a systematic investigation into the formation mechanism of acicular ferrites and the effect of crystal structure on the acicular morphology. This study has therefore focused on these topics in order to discuss the formation mechanism of acicular ferrites from a crystallographic point of view.

1 Experimental Procedures

The experimental materials were 45 steel rods, whose chemical composition is shown in Table 1.

Table 1 Chemical composition of the materials used mass%

C	Si	Mn	P	S	V	Cr	Al	Ti	N
0.47	0.27	0.75	≤0.015	≤0.020	0.08	0.20	0.020	0.012	0.0100

The 45 steel rods were cut into specimens of ϕ3 mm×8 mm. Thereafter, the steel samples were heat treated using a high-temperature confocal scan laser microscope (HTCSLM) with a high accuracy heating/cooling system. These specimens were austenized in argon gas at 1150 ℃ for 10 min, cooled to 500 ℃ at a rate of 30 ℃/min, and then cooled again to room temperature at a rate of 100 ℃/min. The microstructures of the transformed specimens were observed via scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Nital (4 vol. %) was used as an etchant for SEM observation on an S4800 instrument. Thin foil specimens having diameter of 3 mm were prepared for TEM by mechanical thinning followed by argon ion thinning. Conventional TEM observation was performed using JEOL 2010 operated at 200 kV. The composition of the inclusions was identified via TEM-energy dispersive spectroscopy (EDS) and selected area electron diffraction (SAD).

Detailed crystal data for MnS are summarized in Table 2, where, a, b and c are the lattice constants; α, β, and γ are the angles between b and c, a and c, a and b, respectively; and Z is the number of atoms in unit cell. The structures were visualized with the DIAMOND 3.0 program[16].

Table 2 Crystallographic data for MnS

Formula	MnS
Molecular mass	87.010
Crystal system	Cubic
Space group	F-43m (216)
Wavelength, Fe Kα1/nm	0.193597
a/nm	0.56120
b/nm	0.56120
c/nm	0.56120
α/(°)	90.000
β/(°)	90.000
γ/(°)	90.000
Cell volume/nm^3	0.176747
Z	4

2 Results and Discussion

2.1 Characterization

Fig. 1 shows the SEM micrographs of the transformed specimens. The microstructure was dominated by IGF, mainly acicular ferrites. The acicular ferrite has an intragranularly nucleated morphology in which there are multiple impingements between grains (Fig. 1(a)). These acicular ferrites intersect each other and have obviously nucleated on an inclusion (Fig. 1(b)). The needle-like laths of acicular ferrite can nucleate on the inclusion in two different ways: engulfed nucleation or star-like nucleation. In the first case, the inclusions are engulfed mainly by the laths of acicular ferrites. The second type of nucleation creates an interlocking acicular ferrite microstructure.

Fig. 2 shows typical inclusion-induced intragranular ferrites. The inclusions are surrounded by ferrite laths of 3−5 μm in width and 10−20 μm in length. These ferrite laths are radial, symmetrical, and acicular, and the number of ferrite laths nucleated on one inclusion is two, four, and six (Figs. 2(a)−2(c)), respectively. The corresponding angles between