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ARTICLE

A Mathematical Model for Determination of Lamellar Spacing in Materials of Poly-Grain Microstructures

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Abstract: Based on the assumption of spherical grains in polycrystalline materials and the theory of metallography, a mathematical model was developed to calculate the quantitative relationship between apparent and true values of the lamellar spacing cutting through the grain randomly. The results indicate that the grain sizes of most polycrystalline materials are much larger than their lamellar spacings, the ratio of an average apparent value to a true one can be characterized by the corrected coefficient k. The ratio of the apparent lamellar spacing to the grain size reduces from 0.05 to 0.0001, and k increases from 1.5391 to 1.5707, which gradually tends to be $\pi/2$. When the ratio of the apparent lamellar spacing to the grain size is smaller than 0.001, value k can be considered as a constant of $\pi/2$. The amount of work will be decreased adopting the present model to get the true value of lamellar spacing compared with the conventional methods.

Key words: lamellar spacing; quantitative stereology; lamellar structure; mathematical model

The dimension of a microstructure (e.g. lamellar multi-phases resulting from eutectic/nonequilibrium peritectoid reactions etc) or a macrostructure (e.g. polycrystal equiaxed grains etc) is one of the critical characteristic parameter for the solidification or solid-phase-decomposition structures, and often used as an important geometric input-parameter to predict the resultant materials properties. Therefore, many research efforts have been devoted to quantitatively describing the structures of different alloys. However, these investigations primarily focused on the determinations of spatial grain size and its distribution characteristics [1-6]. Microstructures, including lamellae structure, dendrite arm spacing and fibrous structure etc, also have great effects on the material properties, but fewer studies can be found in literatures on more efficient methods for characterizing spatial lamellar microstructures from metallographically measured data [7-13].

For a spatially parallel lamellar microstructure, the observed "lamellar thicknesses" may take a wide spreading variation of the measured data from arbitrarily sectioning plane[14]. The relationships between the randomly sampled data of the lamellar spacing on the microphotograph of the section plane $\lambda^{r}_{\alpha/\beta}$ and the true lamellar thickness $\lambda^{t}_{\alpha/\beta}$ in the three dimensional space of the specimen were derived by Saltykov on the basis of quantitative stereology[7]: $\lambda^{r}_{\alpha/\beta} = 2\lambda^{t}_{\alpha/\beta}$. However, upon using this conventional method, a large amount of the random measurements are usually required due to the technique nature, in order to obtain a reliable datum for the lamellar thickness. Therefore, in literatures the mentioned lamellar thickness may often refer to the apparent spacing [15].

The aim of the present work is to propose a new mathematical model to quantify the lamellar spacing of lamellar microstructure in a polycrystalline specimen. The proposed model and method used a less number of randomly sampled data, therefore by which a more efficient determination was performed for the true lamellar spacing

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$\lambda^t_{\alpha/\beta}$. The present method will be applied to the microstructure of Ti-6Al-4V castings to determine the relationship of the $\alpha+\beta$ lamellar spacing with the cooling rate etc.

1 Modeling Process

1.1 Basic assumptions

Two-phase of an ideal lamellar structure is defined in a spherical grain of a test sample, which is determined by the method of uniform grain size assumption proposed in Ref. [16]. Two-phase lamellar structure is described as α and β lamellae. Fig.1 shows the schematic of the grain cutting randomly by a section plane *i*, and the terms and their corresponding symbols are defined as follows. $\lambda^a_{\alpha/\beta}(i)$ is the apparent lamellar spacing of $(\alpha+\beta)$ on the section plane *i* which can be actually observed on a microphotograph, and $\lambda^t_{\alpha/\beta}$ is the true lamellar spacing in three-dimensional space. The relationship between $\lambda^a_{\alpha/\beta}(i)$ and $\lambda^t_{\alpha/\beta}$ will be investigated. Following assumptions were made during the modeling process.

(1) Any α lamellar thickness was equal to λ^t_α, and β lamella thickness was equals to λ^t_β, α lamella was parallel to β lamella. In this research, we first assumed that $\lambda^t_\alpha \le \lambda^t_\beta$. The true lamellar spacing of $(\alpha+\beta)$ was $\lambda^t_{\alpha/\beta}=\lambda^t_\alpha+\lambda^t_\beta$. α and β lamellae were in a spherical grain with the diameter of d_g.

(2) The origin of three dimensional *x*-*y*-*z* coordinates was the center of the grain, and *y* axis was vertical to the lamella.

(3) Random section plane *i* transited the origin of the coordinate O, and the angles between its normal *n*(*i*) and *x* axis, *y* axis and *z* axis were θ^i_x, θ^i_y, θ^i_z, respectively. Therefore, the normal vector of the plane can be described as: $n(i)=n(i)(\cos\theta^i_x, \cos\theta^i_y, \cos\theta^i_z)$, and the equation of section plane *i* is:

$$\begin{cases} x\cos\theta^i_{\mathrm{x}} + y\cos\theta^i_{\mathrm{y}} + z\cos\theta^i_{\mathrm{z}} = 0 \\ \cos^2\theta^i_x + \cos^2\theta^i_y + \cos^2\theta^i_z = 1 \end{cases} \tag{1}$$

(4) The apparent spacing of lamellar *α*/*β* in section plane *i* was $\lambda^a_{\alpha/\beta}(i)=\lambda^a_\alpha(i)+\lambda^a_\beta(i)$.

1.2 Model analysis

A configuration $(\alpha+\beta)$ lamellar structures and the coordinate system in this investigation are illustrated in Fig.1, as described above for the present modeling analysis. The specific procedures are shown as follows.

First, the intersecting lines of section plane *i* and the interface of lamellae located in $y=-(\lambda^t_\alpha+\lambda^t_\beta)/2$ and $y=(\lambda^t_\alpha+\lambda^t_\beta)/2$ are expressed as L_1 and L_2 respectively, which can be descried with the following equation systems:

$$\begin{cases} x\cos\theta^i_x + y\cos\theta^i_y + z\cos\theta^i_z = 0 \\ y = -\lambda^t_{\alpha/\beta}/2 \end{cases} \tag{2}$$

$$\begin{cases} x\cos\theta^i_x + y\cos\theta^i_y + z\cos\theta^i_z = 0 \\ y = \lambda^t_{\alpha/\beta}/2 \end{cases} \tag{3}$$

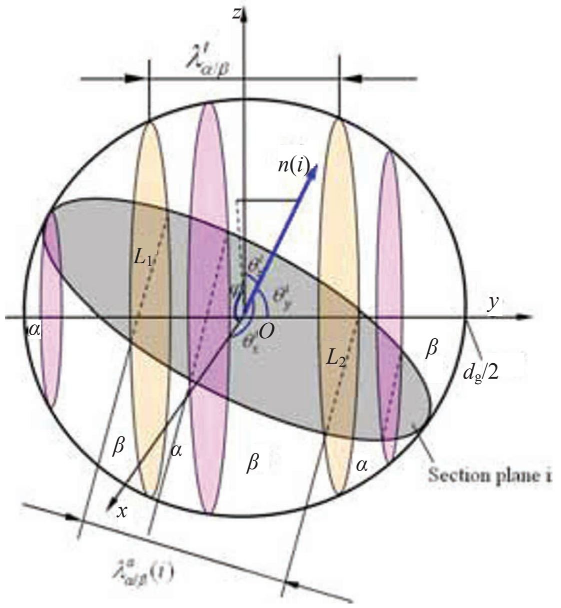

Fig.1 Schematic of a grain cut randomly by a section plane (*i*)

The distance between L_1 and L_2 can be expressed as:

$$\lambda^c_{\alpha/\beta}(i) = \left|\overrightarrow{M_1M_2}\times V_2\right| / \left|V_2\right| \tag{4}$$

where, $\overrightarrow{M_1M_2}$ is the vector of distance between random points of M_1 and M_2 located in L_1 and L_2, respectively. V_2 is the direction vector of L_2.

To simplify the analysis, z_1=0 for the point of $M_1(x_1, y_1, z_1)$ is defined, and then M_1 can be expressed as: $(\lambda^t_{\alpha/\beta}\cos\theta^i_y/2\cos\theta^i_x, -\lambda^t_{\alpha/\beta}/2, 0)$. Likewise, point M_2 can be expressed as: $(-\lambda^t_{\alpha/\beta}\cos\theta^i_y/2\cos\theta^i_x, \lambda^t_{\alpha/\beta}/2, 0)$.

Then the vector $\overrightarrow{M_1M_2}$ is expressed as: $(-\lambda^t_{\alpha/\beta}\cos\theta^i_y/\cos\theta^i_x, \lambda^t_{\alpha/\beta}, 0)$ and $\boldsymbol{V}_2$ can be written as[14] $V_2=n(i)\times n_2$, the normal vector of section plane *i* is $n(i)=n(i)(\cos\theta^i_x, \cos\theta^i_y, \cos\theta^i_z)$; and the normal vector of *α*/*β* lamellar interface at $y=(\lambda^t_\alpha+\lambda^t_\beta)/2$ is n_2=n_2 (0, 1, 0). Then the vector $\boldsymbol{V}_2$ is given in the form as $(-\cos\theta^i_z, 0, \cos\theta^i_x)$. Substituting equation $\overrightarrow{M_1M_2}$ and $\boldsymbol{V}_2$ into equation (4), then the relationship between apparent spacing in section plane *i* and true spacing can be obtained as follows:

$$\lambda^a_{\alpha/\beta}(i) = \lambda^t_{\alpha/\beta} / \left|\sin\theta^i_y\right| \tag{5}$$

1.3 Model solution

Owing to the random distribution of the section plane on the grain of a test sample and the equal probability of its orientation in three-dimension, the statistical relationship between the average apparent lamellar thickness and the true one of the sample can be deduced as follows.

From equation (5), it is obviously known that the factor affecting the relationship between $\lambda^a_{\alpha/\beta}(i)$ and $\lambda^t_{\alpha/\beta}$ is θ^i_y. Theoretically, because the definite value of grain size d_g for a sample is defined, if the section plane *i* is located in the range of only one or less than one $(\alpha+\beta)$ lamella, the apparent lamellar thickness can't be determined correctly, as shown in