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Some theoretical and computational aspects in grain boundaries and triple lines

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Harmonic expansion is a useful tool to analyze the CSL triple junction distribution in a randomly oriented polycrystalline aggregate. By using this approach, a general form of the CSL triple junction distribution could be derived. It makes it possible to calculate—in a very efficient way—the frequency of occurrence of various CSL triple junctions. The accuracy of calculation is confirmed by the estimated frequency for the Σ1-Σ1-Σ1 junctions, which turns out to be in very good agreement with its theoretical value as derived from fully analytical calculation.

1. Introduction

Grain Boundaries and triple junctions—the line along which three grain boundaries meet - are important microstructural elements in polycrystalline materials. The aim of controlling grain boundary (GB) distributions in polycrystalline materials, submitted originally by Watanabe in the context of grain boundary design [1], has drawn significant attention. It has been recently emphasized that, not only the grain boundary distribution, but also the distribution of triple junctions, has to be taken into account since junctions contribute to intergranular degradation resistance [2] and also have a significant impact on grain boundary migration [3–6]. Recent experimental and theoretical work has revealed that the various properties of individual grain junctions, including energy, diffusivity, corrosion, mobility, etc., are strongly structure-dependent [7]. Three complementary models have been the object of special attention for the interpretation of the triple junction structure: the Coincident Site Lattice (CSL) method [8], the Coincident Axial Direction (CAD) approach [9] and the I/U line treatment [10, 11]. This paper is concerned with the calculation of the triple junction character distribution of randomly oriented cubic crystals on the basis of the CSL model. In the specific case of Σ1-Σ1-Σ1 junctions, the corresponding occurrence frequency has been derived as a close formula by means of fully analytical calculations. The results obtained are of importance to analyze CSL triple junctions in real materials.

2. Methodology

2.1. Description of a CSL triple junction

First, we consider an exact CSL misorientation g_Σ in matrix representation. Due to symmetry, this misorientation corresponds to K_Σ equivalent elements of the rotation group SO(3). Let C denote the subgroup of crystal point symmetries containing only proper rotations. K_Σ can be established easily by counting the number of different elements within the double coset [12]

$$\left\{g_\Sigma^{\mathrm{k}}\right\} = \left\{g \in \mathrm{SO}(3) \mid g = c_{\mathrm{m}} g_\Sigma c_{\mathrm{n}} \text{ or } g = c_{\mathrm{m}} g_\Sigma^{-1} c_{\mathrm{n}},\ c_{\mathrm{m}}, c_{\mathrm{n}} \in \mathrm{C}\right\}. \quad (1)$$

By convention, a grain boundary is assigned to a certain Σ CSL type if its misorientation g is sufficiently close to at least one of the elements of the $\{g_\Sigma^{\mathrm{k}}\}$. Brandon's criterion [13], i.e.

$$\Delta\theta_\Sigma = 15^\circ\ \Sigma^{-1/2}, \quad (2)$$

has often been used to determine the maximum allowable angular deviation $\Delta\theta_\Sigma$ for certain CSL boundaries. However, Palumbuo and Aust have recently proposed a more selective criterion [14]

$$\Delta\theta_\Sigma = 15^\circ\ \Sigma^{-5/6}. \quad (3)$$

Let us now consider a triple junction where grain boundaries 1, 2, 3 meet (Fig. 1). The misorientation geometry of the triple junction is governed by the following relationship:

$$g_1 g_2 g_3 = I, \quad (4)$$

where g_{i} ($i = 1, 2, 3$) are the misorientation matrices of three co-joining grain boundaries and I is the identity matrix.

Similarly, the triple junction is classified as a CSL triple junction when all involved boundaries are low Σ

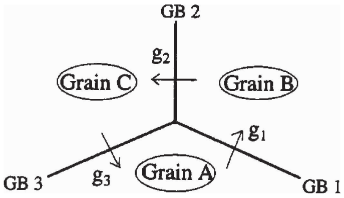

Figure 1 Schematic representation of a triple junction geometry.

CSL types. This can be formally described as

$$\begin{aligned} g_1 \in \Sigma a &\leftrightarrow \exists_{\mathrm{i}} \mid \Omega\big(g_1\big(g^{\mathrm{i}}_{\Sigma_a}\big)^{-1}\big) \le \Delta\theta_{\Sigma a} \\ g_2 \in \Sigma b &\leftrightarrow \exists_{\mathrm{j}} \mid \Omega\big(g_2\big(g^{\mathrm{j}}_{\Sigma_b}\big)^{-1}\big) \le \Delta\theta_{\Sigma b}, \\ g_3 \in \Sigma c &\leftrightarrow \exists_{\mathrm{k}} \mid \Omega\big(g_3\big(g^{\mathrm{k}}_{\Sigma_c}\big)^{-1}\big) \le \Delta\theta_{\Sigma c} \end{aligned} \tag{5}$$

where $\Omega(g)$ is the angle of the rotation g.

2.2. The series expansion approach

For a randomly oriented polycrystal, the frequency of occurrence of CSL triple junctions is given by a double integral

$$F_{\Sigma a-\Sigma b-\Sigma c} = N_{\Sigma a-\Sigma b-\Sigma c} \iint_\tau dg_1 dg_2, \qquad \tau\colon \begin{array}{l} g_1 \in \Sigma a \\ g_2 \in \Sigma b \\ g_2 g_1 \in \Sigma c \end{array} \tag{6}$$

where $N_{\Sigma a-\Sigma b-\Sigma c}$ is the number of possible geometrical configurations belonging to the same family Σa-Σb-Σc, i.e. 1 for $\Sigma a = \Sigma b = \Sigma c$, 3 for $\Sigma a = \Sigma b \neq \Sigma c$ and 6 for $\Sigma a \neq \Sigma b \neq \Sigma c$. To perform the above integration, we introduce the characteristic function $I_\Sigma(g)$ of the set of rotations whose angle is smaller than $\Delta\theta_\Sigma$ defined as

$$I_\Sigma(g) = \begin{cases} 1 & \Omega\big(g\big(g^{\mathrm{i}}_\Sigma\big)^{-1}\big) \le \Delta\theta_\Sigma, \\ & \qquad\qquad i = 1, 2, \ldots, K_\Sigma. \\ 0 & \Omega\big(g\big(g^{\mathrm{i}}_\Sigma\big)^{-1}\big) > \Delta\theta_\Sigma \end{cases} \tag{7}$$

Such a symmetrised function may be represented in the form of a series [15]:

$$I_\Sigma(g) = \sum_{l=0}^{\infty} \sum_{\alpha=1}^{M(l)} \sum_{\beta=1}^{M(l)} I_l^{\alpha\beta}(\Sigma)\, \ddot{T}_l^{\alpha\beta}(g) \tag{8}$$

with the series expansion coefficients

$$I_l^{\alpha\beta}(\Sigma) = (2l+1) \oint I_\Sigma(g)\, \ddot{T}_l^{*\alpha\beta}(g)\, dg, \tag{9}$$

where $\ddot{T}_l^{\alpha\beta}(g)$ are generalised spherical harmonics satisfying the crystal symmetries on both sides and the asterisk denotes the complex conjugate. We have proven for the $I_l^{\alpha\beta}(\Sigma)$ coefficients that

$$I_l^{\alpha\beta}(\Sigma) = \frac{K_\Sigma}{2\pi} W_l(\Delta\theta_\Sigma)\big[\, \ddot{T}_l^{*\alpha\beta}(g_\Sigma) + \ddot{T}_l^{*\alpha\beta}(g_\Sigma^{-1})\big] \tag{10}$$

with

$$W_l(\Delta\theta_\Sigma) = \begin{cases} \Delta\theta_\Sigma - \sin(\Delta\theta_\Sigma) & l = 0 \\ \sin(l\Delta\theta_\Sigma)/l - \sin \\ \quad \times [(l+1)\Delta\theta_\Sigma]/(l+1) & l > 0 \end{cases}. \tag{11}$$

The expression (6) can be written as

$$F_{\Sigma a-\Sigma b-\Sigma c} = N_{\Sigma a-\Sigma b-\Sigma c} \oiint I_{\Sigma a}(g_1) I_{\Sigma b} \times (g_2) I^*_{\Sigma c}(g_2 g_1)\, dg_1 dg_2. \tag{12}$$

If we rewrite I_Σ(g) as defined in (8) into (12) and take into account the orthonormality relation of the generalized spherical harmonics, we obtain

$$F_{\Sigma a-\Sigma b-\Sigma c} = N_{\Sigma a-\Sigma b-\Sigma c} \sum_{l=0}^{\infty} \frac{1}{(2l+1)^2} \times \sum_{\alpha,\beta,\gamma=1}^{M(l)} I_l^{\alpha\beta}(\Sigma a) I_l^{\gamma\alpha}(\Sigma b) I_l^{\beta\gamma}(\Sigma c). \tag{13}$$

Moreover, we restrict ourselves to those CSL junctions with $\Sigma \le 29$.

Under that condition, the following formula holds:

$$\{c_{\mathrm{i}} g_\Sigma c_{\mathrm{j}},\, c_{\mathrm{i}}, c_{\mathrm{j}} \in C\} = \big\{c_{\mathrm{m}} g_\Sigma^{-1} c_{\mathrm{n}},\, c_{\mathrm{m}}, c_{\mathrm{n}} \in C\big\}. \tag{14}$$

Hence,

$$I_l^{\alpha\beta}(\Sigma) = \frac{K_\Sigma}{\pi} W_l(\Delta\theta_\Sigma)\, \ddot{T}_l^{*\alpha\beta}(g_\Sigma). \tag{15}$$

We further obtain

$$\begin{aligned} F_{\Sigma a-\Sigma b-\Sigma c} &= K_{\Sigma a} K_{\Sigma b} K_{\Sigma c} N_{\Sigma a-\Sigma b-\Sigma c} \\ &\quad \times \sum_{l=0}^{\infty} \frac{W_l(\Delta\theta_{\Sigma a}) W_l(\Delta\theta_{\Sigma b}) W_l(\Delta\theta_{\Sigma c})}{(2l+1)^2 \pi^3} \\ &\quad \times \sum_{\alpha,\beta,\gamma=1}^{M(l)} \ddot{T}_l^{\alpha\beta}(g_{\Sigma a})\, \ddot{T}_l^{\gamma\alpha}(g_{\Sigma b})\, \ddot{T}_l^{\beta\gamma}(g_{\Sigma c}). \end{aligned} \tag{16}$$

The following relation is valid

$$\begin{aligned} &\sum_{\alpha,\beta,\gamma=1}^{M(l)} \ddot{T}_l^{\alpha\beta}(g_{\Sigma a})\, \ddot{T}_l^{\gamma\alpha}(g_{\Sigma b})\, \ddot{T}_l^{\beta\gamma}(g_{\Sigma c}) \\ &\quad = \frac{1}{N_c^3} \sum_{i,j,k=1}^{N_c} \chi_l(\Omega(c_i g_{\Sigma a} c_j g_{\Sigma b} c_k g_{\Sigma c})), \end{aligned} \tag{17}$$

where N_c is the order of the subgroup C, i.e. $N_c = 24$ for the cubic symmetry, and $\chi_l(\omega)$ are the trace—or character—of the representation of the rotation group. They take on the explicit form

$$\chi_l(\omega) = \sin[(2l+1)\omega/2]/\sin(\omega/2). \quad (18)$$

Thus, (15) can also be written as

$$F_{\Sigma a-\Sigma b-\Sigma c} = \frac{K_{\Sigma a}K_{\Sigma b}K_{\Sigma c}N_{\Sigma a-\Sigma b-\Sigma c}}{\pi^3 N_c^3} \times \sum_{l=0}^{\infty} \frac{W_l(\Delta\theta_{\Sigma a})W_l(\Delta\theta_{\Sigma b})W_l(\Delta\theta_{\Sigma c})}{(2l+1)^2} \times \sum_{\alpha,\beta,\gamma=1}^{N_C} \chi_l(\Omega(c_i g_{\Sigma a} c_j g_{\Sigma b} c_k g_{\Sigma c})). \quad (19)$$

The expressions (19) or (16)—or the more general expression (13)—provide an analytical solution for (6). For practical calculation, the series expansion has to be truncated at a finite rank l_{max}, which, in turn, determines the accuracy. The terms of type $W_l(\Delta\theta_{\Sigma a})$ in (19) decrease very rapidly as l increases. This suggests that a high numerical accuracy may be obtained at a relatively low l_{max} value.

As a special case, we consider the frequency of Σ1-Σ1-Σ1 triple junctions. This type of junctions is of particular interest because it always builds an I-line displaying special properties [16, 17]. Substituting $g_{\Sigma a} = g_{\Sigma b} = g_{\Sigma c} = I$, $N_{\Sigma a-\Sigma b-\Sigma c} = 1$ and $K_{\Sigma 1} = 24$ in (19), we obtain

$$F_{\Sigma 1-\Sigma 1-\Sigma 1} = \frac{24^3}{\pi^3} \sum_{l=0}^{\infty} \frac{M(l)}{(2l+1)^2} [W_l(\delta)]^3 \quad (20)$$

with

$$M(l) = \frac{1}{24} \sum_{i=1}^{N_C} \chi_l(\Omega(c_i)), \quad \delta = \Delta\theta_{\Sigma 1} = 15^\circ. \quad (21)$$

3. Results and discussion

Table I shows the fractions of CSL triple-junction distributions in randomly oriented materials for some CSL triple junctions obtained according to (13) in which the series expansion was truncated at $l = 44$.

An explicit expression for the $F_{\Sigma 1-\Sigma 1-\Sigma 1}$ has also been found by straightforward—though rather tedious—fully analytical calculation, as an alternative to the series expansion. This method implies that the region and limits of the integration involved in (6) are taken into account. Detailed proof of this is provided in Appendix 1. We are content with giving here only the final form:

$$F_{\Sigma 1-\Sigma 1-\Sigma 1} = \frac{144}{\pi^2}\left(14 + 3\delta^2 + 18\cos\delta - 6\delta\sin\delta - 32\cos^3\frac{\delta}{2}\right). \quad (22)$$

It can be observed that the value for Σ1-Σ1-Σ1 triple junctions obtained by using the harmonic expansion approximation fits well with the theoretical fraction (0.024356%) directly derived from the analytical exact expression (22). This suggests that the truncation error is negligible in the procedure concerned.

Fortier *et al*. [18] have evaluated the CSL triple junction distributions in randomly oriented and in fiber-textured materials by computer simulation. As reported, the fractions of Σ1-Σ1-Σ1, Σ1-Σ3-Σ3 and Σ3-Σ3-Σ9 triple junctions in a randomly oriented distribution were about 0.04%, 0.015% and 0.005%, respectively. The discrepancy with the present values may probably be related to an insufficient sampling in their calculations.

It was shown in Table II that, when using extended sampling applying a variant of the Monte-Carlo simulation method designed to exclude any rejection, we can achieve a degree of accuracy comparable to that of the series expansion approach. But Monte-Carlo methods generally impose a much longer computation time, which—in certain cases—nearly invalidates the procedure. Thus, the series expansion method appears as more powerful for the type of study reported in this paper.

TABLE I Frequencies of occurrence of various CSL triple junctions in randomly oriented cubic crystals, as calculated following the harmonic expansion method (Equation 13)

Type	Frequency % according to Palumbo & Aust's criterion	Frequency % according to Brandon's criterion	Frequency % according to Fortier *et al*. [19]	Frequency % theoretical value, derived directly from (22)
Σ1-Σ1-Σ1	0.024366	0.024366	0.04	0.024356
Σ1-Σ3-Σ3	0.002567	0.022606	0.015	
Σ1-Σ5-Σ5	0.000397	0.009691		
Σ1-Σ7-Σ7	0.000086	0.003632		
Σ1-Σ9-Σ9	0.000040	0.002583		
Σ1-Σ27a-Σ27a	0.000000	0.000111		
Σ1-Σ27b-Σ27b	0.000000	0.000222		
Σ3-Σ3-Σ9	0.000360	0.009143	0.005	
Σ3-Σ9-Σ27a	0.000006	0.001249		
Σ3-Σ9-Σ27b	0.000012	0.002270		

TABLE II Frequencies of occurrence of various CSL triple junctions in randomly oriented cubic crystals calculated with the Monte-Carlo method

Type	Frequency % according to Palumbo and Aust's criterion	Frequency % according to Brandon's criterion
Σ1-Σ1-Σ1	0.024110	0.023050
Σ1-Σ3-Σ3	0.002800	0.021610
Σ1-Σ5-Σ5	0.000360	0.008790
Σ1-Σ7-Σ7	0.000080	0.003490
Σ1-Σ9-Σ9	0.000030	0.002550
Σ1-Σ27a-Σ27a	0.000000	0.000100
Σ1-Σ27b-Σ27b	0.000000	0.000220
Σ3-Σ3-Σ9	0.000430	0.008170
Σ3-Σ9-Σ27a	0.000000	0.000890
Σ3-Σ9-Σ27b	0.000010	0.002230

Except for the Σ1-Σ1-Σ1 frequency, with the maximum allowable angular deviations $\Delta\theta_\Sigma$ determined according to respectively Brandon's criterion and Palumbo and Aust's criterion, the results are quite different. Indeed, the more selective Palumbo and Aust's $\Delta\theta_\Sigma$ criterion yields—with the exception of the Σ1-Σ1-Σ1 triple line—noticeably smaller CSL triple line frequencies than the Brandon's criterion.

We should bear in mind that the series expansion method has also been applied successfully to the study of the influence of the crystallographic texture on the CSL triple junction distributions in both peak-type and fiber-type ({001}, {110}, {111}) textured materials [19], where the basic assumption was made that there was no orientation correlation in adjacent grains. As was shown in this paper, the fractions of Σ1-Σ1-Σ1 triple junctions increase monotonously with the increasing texture sharpness.

4. Concluding remarks

The basic purpose of this study is to present a theoretical approach to the CSL triple junction distribution in a randomly oriented polycrystal. The use of harmonic expansion yields a mathematically convenient formulation, enabling to calculate the frequencies of CSL triple junctions with adequate accuracy. The results obtained are expected to become a useful reference to various measured distributions. Furthermore, the present mathematical treatment may be extended to the more general case of textured polycrystals.

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Appendix 1

An explicit expression for the $F_{\Sigma1-\Sigma1-\Sigma1}$ can be derived by a straightforward but tedious examination of the region and limits of the integration involved in (6). From (6), we obtain

$$F_{\Sigma1-\Sigma1-\Sigma1} = \iint_\tau dg_1 dg_2 \qquad \tau: \begin{array}{l} g_1 \in \Sigma a \\ g_2 \in \Sigma b \\ g_2 g_1 \in \Sigma c \\ g_1' = g_1 c_i \\ g_2' = c_j g_2 \end{array}$$

$$= \sum_{i=1}^{N_c}\sum_{j=1}^{N_c}\sum_{k=1}^{N_c} \iint_{\substack{\Omega(g_1 c_i)\le\delta \\ \Omega(g_2 c_j)\le\delta \\ \Omega(g_3 c_k)\le\delta}} dg_1 dg_2$$

$$= \sum_{i,j=1}^{N_c}\sum_{m=1}^{N_c} \iint_{\substack{\Omega(g_1')\le\delta \\ \Omega(g_2')\le\delta \\ \Omega(g_2' g_1' c_m)\le\delta}} dg_1' dg_2'$$

$$= \sum_{m=1}^{N_c} N_c^2 \iint_{\substack{\Omega(g_1)\le\delta \\ \Omega(g_2)\le\delta \\ \Omega(g_2 g_1 c_m)\le\delta}} dg_1 dg_2 \tag{A1}$$

We define a characteristic function

$$f_\delta(g) = \begin{cases} 1 & \Omega(g) \le \delta \\ 0 & \Omega(g) > \delta \end{cases}, \tag{A2}$$

Then,

$$\sum_{k=1}^{N_c} N_c^2 \iint_{\substack{\Omega(g_1)\le\delta \\ \Omega(g_2)\le\delta \\ \Omega(g_2 g_1 c_m)\le\delta}} dg_1 dg_2$$

$$= \iint_{\Omega(g_2 g_1 c_m)\le\delta} f_\delta(g_1) f_\delta(g_2)\, dg_1 dg_2 \tag{A3}$$

$$= \int_{|g c_m|\le\delta} h(g)\, dg \quad g = g_2 g_1$$

$$h(g) = \oint_{SO(3)} f_\delta(g_1) f_\delta(g g_1^{-1})\, dg_1 \tag{A4}$$

As proven in [20], the orthogonal rotation matrix can be written as:

$$g_1 = e^{\omega_1 \vec{n}_1}$$
$$g = e^{\omega \vec{n}}. \tag{A5}$$

$$h(g) = \frac{2}{\pi}\int_0^\pi \sin^2\frac{\omega_1}{2} \times \left[\oint_{S_2} f_\delta\left(e^{\omega_1 \vec{n}_1}\right) f_\delta\left(e^{\omega\vec{n}} e^{-\omega_1 \vec{n}_1}\right) d\vec{n}_1\right] d\omega_1 \tag{A6}$$

We define

$$e^{\omega\vec{n}} \cdot e^{-\omega_1 \vec{n}_1} = e^{\hat{\omega}\vec{\hat{n}}}. \tag{A7}$$

As the characteristic function depends only of the angle and not of the axis of the rotation, $f_\delta(e^{\omega_1\vec{n}_1}) = f_\delta(e^{\omega_1\vec{k}_1})$, with $\vec{k}_1$ being fixed, we get

$$h(g) = \frac{2}{\pi}\int_0^\pi f_\delta\left(e^{\omega_1\vec{k}_1}\right) \times \sin^2\frac{\omega_1}{2}\left[\oint_{S_2} f_\delta\left(e^{\hat{\omega}\vec{\hat{n}}}\right) d\vec{n}_1\right] d\omega_1. \quad \text{(A8)}$$

where

$$\oint_{S_2} f_\delta\left(e^{\hat{\omega}\vec{\hat{n}}}\right) d\vec{n}_1 = \frac{1}{4\pi}h(g)\int_0^\pi \sin\theta d\theta \int_0^{2\pi} f_\delta\left(e^{\hat{\omega}\vec{\hat{k}}}\right) d\varphi = \frac{1}{2}\int_0^\pi f_\delta\left(e^{\hat{\omega}\vec{\hat{k}}}\right)\sin\theta d\theta = \frac{1}{2}\int_{|\omega-\omega_1|}^{\omega+\omega_1} f_\delta\left(e^{\hat{\omega}\vec{\hat{k}}}\right)\frac{\sin\frac{\hat{\omega}}{2}d\hat{\omega}}{2\sin\frac{\omega}{2}\sin\frac{\omega_1}{2}} = \frac{1}{4\sin\frac{\omega}{2}\sin\frac{\omega_1}{2}}\int_{|\omega-\omega_1|}^{\omega+\omega_1} f_\delta\left(e^{\hat{\omega}\vec{\hat{k}}}\right)\sin\frac{\hat{\omega}}{2}d\hat{\omega} \quad \text{(A9)}$$

When δ is small enough, there is no risk of overlapping of the equivalent regions in the Euler space, so that

$$\sum_{k=1}^{N_c}\int_{|gc_m|\le\delta} h(g)\,dg = \int_{|g|\le\delta} h(g)\,dg \quad \text{(A10)}$$

So we obtain according to a tricky subdivision of the integration domain of the double integral

$$F_{\Sigma1-\Sigma1-\Sigma1} = N_c^2\int_{|g|\le\delta} h(g)\,dg = \frac{N_c^2}{\pi^2}\int_0^\delta \sin\frac{\omega}{2}d\omega\int_0^\pi \sin\frac{\omega}{2}d\omega = \frac{N_c^2}{\pi^2}\int_0^\delta \sin\frac{\omega}{2}d\omega\left\{\int_0^{\delta-\omega}\sin\frac{\omega_1}{2}d\omega_1 \times \int_{|\omega-\omega_1|}^{\omega+\omega_1}\sin\frac{\hat{\omega}}{2}d\hat{\omega} + \int_{\delta-\omega}^{\delta}\sin\frac{\omega_1}{2}d\omega_1 \times \int_{|\omega-\omega_1|}^{\delta}\sin\frac{\hat{\omega}}{2}d\hat{\omega}\right\}$$

$$= \frac{N_c^2}{\pi^2}\left(\frac{3}{4}\delta^2 - 1 + 9\cos^2\frac{\delta}{2} - 8\cos^3\frac{\delta}{2} - \frac{3}{2}\delta\sin\delta\right) = \frac{144}{\pi^2}\left(14 + 3\delta^2 + 18\cos\delta - 6\delta\sin\delta - 32\cos^3\frac{\delta}{2}\right).$$

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