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The particle distribution functions and applications

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The new generalized logarithmic equation defined by four parameters, called LG4, was formulated and proposed for describing particle size and shape distributions. For special choice of the parameters the LG4 was reduced to the logarithmic distribution LG2 defined by two parameters which permits the selection of mean value of the distribution as the size parameter appears explicitly in the distribution function. The LG2 has been suggested as a model for size and shape distributions of the particles (the "fourth state of matter" according to Heywood's definition) as, for example, the metallic and ceramic particles which attract a good deal of public attention as new promising high-performance materials for magnetic materials and then chemical catalysts, sintering promoting materials, sensors, etc. The shape and similarity of the particle for some purposes are very important. Total volume, total surface or any other useful property of the sample, may be related to shape and size of individual particles. If all particles are geometrically similar, all the subsequent treatment is simplified substantially in terms of shape. By introducing *the shape parameter* of the particle*, the generalized similarity* and *the elliptic factor* of the assembly of particles the application of the LG2 for the study of the shape distribution of the projected $Nd_2Fe_{14}B$ particles is referred in this paper.

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1. Introduction

A lot of various materials can be used as a coating, depending on the future use of optical fiber with composite magnetic coating. Magnetic field sensors based on optical fibers with composite coating are modern materials with wide range of application in high sensitive measuring techniques in nearly all parts of engineering. Optical fiber with modified coating polymer – magnetic powder can be used as a sensing element and the element of magnetometer on the basis of optical fibers. Composite coating with magnetic powder can be used as a locator for optical fiber. There are a lot of applications of these magnetic materials in biomagnetic systems, in medicine, diagnostics, etc. The main study topic of many scientific institutions is investigation of dependence of modified optical fiber as a magnetic field sensing element on coating process. This topic was realized through characterization of components which are in the composite coating. Special attention was paid to the characterization and chosing of magnetic powder of optimal quality which will allow the best sensitivity and reversibility of modified optical fiber and the whole sensing element. Composite coating with magnetic powder of high-coercive magnetic materials based on Neodymium Iron Boron (Nd-Fe-B) attracts a good deal of public attention as new promising high-performance materials. In recent time the study topic of many scientific institutions throughout the world is the process of obtaining high-coercive magnetic materials based on Nd-Fe-B. In order to fulfill economic requests for the lowest price, the optimization weight percent of magnetic powder in the composite coating are of great importance. Besides that, the particle size and shape distributions together with the microstructure of $Nd_2Fe_{14}B$ are significant for magnetic properties. They have also considerable influence on homogeneity of polymer – magnetic medium suspension. Therefore, it was specially important to find particle size and shape distributions of magnetic powder [1-6]. Experimental particle sizes often obey a lognormal size distribution and other logarithmically skewed distributions, besides Rosin-Rammler, Nukiyama-Tanasawa distributions, etc.[7-20]. In earlier distribution functions studies of the authors, a number of properties of the general family of logarithmically skewed distributions (the new generalized logarithmic distribution defined by four parameters, LG4) have been described. In previous works, the authors have presented analyses of previously developed distributions, development and application of the logarithmic distribution defined by two parameters (LG2), and comparisons of the various distribution functions with experimental data. The authors showed in details that previously applied logarithmic distribution equations, developed by other authors, can be obtained from the LG4 for special choice of its parameters and that the LG2 (special case of the LG4) better fitted to the experimental data than the well-known lognormal and logarithmic distribution defined by one parameter LG1 which are also special cases of the LG4. The LG2 distribution, the mean value of which appears explicitly in its probability density equation, has been suggested as a model for size and shape distributions of the particles [11,14,18].

In this paper the authors continue with the application of the LG2 for the study of the shape distribution introducing *the shape parameter* and *the generalized similarity*. Using the longest and shortest dimension distributions of projected particles, it was found the distribution of the particle *shape parameter*. An approach to the study of the particles *generalized similarity* was performed. The deviation of the particle shape from the elliptical shape and the particle outline smoothness was analyzed. *The elliptic factor* of an assembly of particles is also defined, and the LG2 is applied to estimate this factor. The LG4 and LG2 equations can be applied to a wide variety of experimental data. As an illustration of the proposed model, the particle shape analyses of the $Nd_2Fe_{14}B$ magnetic powder are performed.

2. The LG4 and LG2 logarithmic distributions

Let us introduce the new distribution defined by four parameters (LG4) (Appendix A, A1-A6) with the probability density function (PDFLG4) [11,18]:

$$f_{LG4\left(p,x_{1p}x_{2p},\zeta_p\right)}(x)=f_p(x)=\frac{x^p\exp\left[-\dfrac{\left(\ln x-\ln x_{1p}\right)\left(\ln x-\ln x_{2p}\right)}{2\zeta_p^2}\right]}{x_{1p}^{p+1}\zeta_p\sqrt{2\pi}\ \exp\left\{\dfrac{\left[2(p+1)\zeta_p^2-\ln\left(x_{1p}/x_{2p}\right)\right]^2}{8\zeta_p^2}\right\}}, \tag{2.1}$$

where p, x_{1p}, x_{2p} and ζ_p are the parameters of this distribution.

The mean value of the PDFLG4 is (A7)

$$\bar{x}_p=\sqrt{x_{1p}x_{2p}}\exp\left(\frac{(2p+3)\zeta_p^2}{2}\right). \tag{2.2}$$

The standard deviation of the PDFLG4 is (A8-A11)

$$\sigma_p=\sqrt{x_{1p}x_{2p}}\exp\left(\frac{2p+3}{2}\zeta_p^2\right)\sqrt{\exp\left(\zeta_p^2\right)-1}. \tag{2.3}$$

The geometric mean of PDFLG4 is (Appendix B)

$$x_g=\sqrt{x_{1p}x_{2p}}\exp\left[(p+1)\zeta_p^2\right]. \tag{2.4}$$

On combining (2.2) and (2.4) we obtain

$$x_g=\bar{x}_p\exp\left(-\frac{\zeta_p^2}{2}\right). \tag{2.5}$$

Note that the parameter p does not appear in (2.5). If $p=-3/2$, the exponential terms in (2.2) and (2.3) vanish so the mean value is reduced to $\sqrt{x_{1p}x_{2p}}$ and the standard deviation becomes $\sqrt{x_{1p}x_{2p}}\sqrt{\exp\left(\zeta_p^2\right)-1}$. Hence, the variation of ζ_p will change the shape of the distribution curve while the mean value maintains invariant. Thus, it can be written $x_{2p}=\left(\bar{x}_p\right)^2/x_{1p}$. Let us denote $\bar{x}_p=\bar{x}$, $x_{1p}=x_1$, $x_{2p}=x_2=\bar{x}^2/x_1$, $\zeta_p=\zeta$ and $\sigma_p=\sigma$. Then, the PDFLG4 becomes the probability density function defined by two parameters (PDFLG2):

$$f(x)=\frac{x^{-3/2}\exp\left[-\dfrac{\left(\ln x-\ln x_1\right)\left(\ln x-\ln\left(\bar{x}^2/x_1\right)\right)}{2\zeta^2}\right]}{x_1^{-1/2}\zeta\sqrt{2\pi}\exp\left\{\dfrac{\left[\zeta^2+\ln\left(x_1^2/\bar{x}^2\right)\right]^2}{8\zeta^2}\right\}}. \tag{2.6}$$

Substituting $p=-3/2$ ($\zeta_p=\zeta$, $\sigma_p=\sigma$) into (2.3) and supposing $\zeta^2<<1$ ($\exp\left(\zeta^2\right)\approx 1+\zeta^2$) we have

$$\sigma\approx\bar{x}\zeta\text{, i. e. }\zeta\approx\frac{\sigma}{\bar{x}}. \tag{2.7}$$

Therefore, under assumption that a distribution is sufficiently narrow, the parameter ζ could be a measure of the degree of variation (or spread) of the distribution.

2.1. Analysis of the real powder ($Nd_2Fe_{14}B$) as an illustration of developed model

The particles of $Nd_2Fe_{14}B$ were analyzed by scanning electron microscopy (SEM) with spectrometer type «Philips XL-30 DX 4i» and light microscope «Reichert» type POLYVAR-MET with the quantitative image analyzer Q500MC-Leica with software Qwin (1997) [5]. The distributions of geometrical equivalent dimensions of selected samples defined in projection (the longest R and shortest r dimensions and the area S) were examined and determined. Note geometrical equivalent dimensions are defined in projection and therefore the particle size and shape are, in fact, size and shape of projected particle. In order to simplify, "projected particles" are often termed - "particles" in this paper. At the beginning of the investigation, particles were in the form of small plates (in space) having linear dimensions of about $100-150\mu m$. The projection of these $Nd_2Fe_{14}B$ particles were polygon in shape. The particles had tendency to become elliptic by grinding. After 2.5 hours of grinding, the particles were of optimal size for the composite coating of sensor element and the forms of small plates were mostly elliptic. A large number $(n=700)$ of these particles (made from the origin particles) were analyzed. It was obtained the empirical distributions of: the longest dimension R, the shortest dimensions r and the surface area S of projected particles. The mean, minimum and maximum values of those parameters are given in Table 1. The distribution LG2 will be fitted to the empirical distributions of geometrical equivalent dimensions of selected samples defined in projection (the longest R and shortest r dimensions and the area S) using the OriginPro 7.5 in order to obtain the unknown parameters.

Table 1. The experimental data for the particles of $Nd_2Fe_{14}B$ [5].

	Mean value	Minimum	Maximum
Longest dimension (R), μm	$\bar{R}=0.91448$	$R_{min}=0.49020$	$R_{max}=1.54695$
Shortest dimension (r), μm	$\bar{r}=0.68922$	$r_{min}=0.1634$	$r_{max}=1.4756$
Surface (S), μm^2	$\bar{S}=0.49142$	$S_{min}=0.1335$	$S_{max}=1.2425$

To be fitted to the $Nd_2Fe_{14}B$ particles empirical distributions (of R, r and S, respectively) the PDFLG2 takes the forms:

$$F_{LG2}(R)=F(R)=\frac{R^{-3/2}\exp\left[-\frac{(\ln R-\ln R_1)\left(\ln R-\ln\left(\bar{R}^2/R_1\right)\right)}{2\delta^2}\right]}{R_1^{-1/2}\delta\sqrt{2\pi}\exp\left\{\frac{\left[\delta^2+\ln\left(R_1^2/\bar{R}^2\right)\right]^2}{8\delta^2}\right\}}, \tag{2.1.1}$$

$$f_{LG2}(r)=f(r)=\frac{r^{-3/2}\exp\left[-\frac{(\ln r-\ln r_1)\left(\ln r-\ln\left(\bar{r}^2/r_1\right)\right)}{2\rho^2}\right]}{r_1^{-1/2}\rho\sqrt{2\pi}\exp\left\{\frac{\left[\rho^2+\ln\left(r_1^2/\bar{r}^2\right)\right]^2}{8\rho^2}\right\}} \tag{2.1.2}$$

and

$$G_{LG2}(S)=G(S)=\frac{S^{-3/2}\exp\left[-\frac{(\ln S-\ln S_1)\left(\ln S-\ln\left(\bar{S}^2/S_1\right)\right)}{2w^2}\right]}{S_1^{-1/2}w\sqrt{2\pi}\exp\left\{\frac{\left[w^2+\ln\left(S_1^2/\bar{S}^2\right)\right]^2}{8w^2}\right\}} \tag{2.1.3}$$

The parameters of distribution functions are obtained from a best fit to the experimental data by using the OriginPro 7.5 program based on the Levenberg-Marquardt algorithm: $\delta=0.28713$, $\rho=0.32992$ and $w=0.50502$. The values of the corresponding Chi^2/DoF are: $\left(\mathrm{Chi}^2/\mathrm{DoF}\right)_{\mathrm{LG2,R}}=0.05059\mu\mathrm{m}^{-2}$, $\left(\mathrm{Chi}^2/\mathrm{DoF}\right)_{\mathrm{LG2,r}}=0.00600\mu\mathrm{m}^{-2}$, $\left(\mathrm{Chi}^2/\mathrm{DoF}\right)_{\mathrm{LG2,S}}=0.0188\mu\mathrm{m}^{-4}$. The empirical curves together with corresponding fitted density functions are shown in Figs. 1-3.

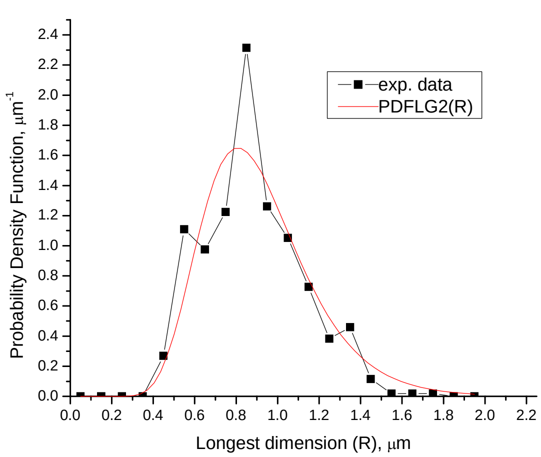

Fig. 1. The PDFLG2 curves fitted to the empirical distribution of the particle longest dimension.

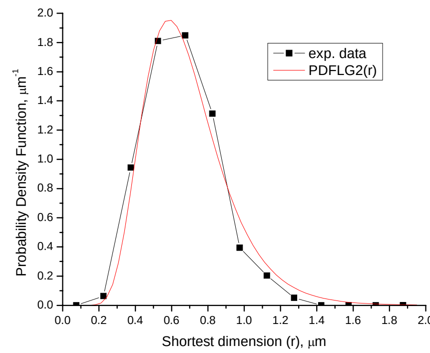

Fig. 2. The PDFLG2 curves fitted to the empirical distribution of the particle shortest dimension.

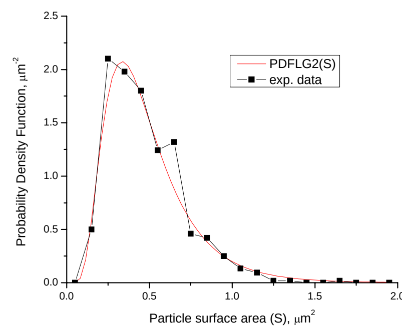

Fig. 3. The PDFLG2 curves fitted to the empirical distribution of the particle surface.

3. The shape parameter distribution of the particles

Consider an assembly of n particles. Let us define *the shape parameter* of the i th $(i=1,2,...,n)$ particle as the longest/shortest dimension ratio $\xi_i=r_i/R_i$, $(0<\xi_i\le 1)$. Let two particles be mutually *generally similar* if they have the same *shape parameter*. Now we will determine *the shape parameter* distribution based on the distributions of the longest and shortest dimensions of the particles. If the probability density functions of the longest and shortest dimensions distributions are $F(R)$ and $f(r)$, respectively, the probability that any particle has $\xi(=r/R)$ in an interval $(\xi,\xi+d\xi)$ $(0<\xi\le 1)$ is

$$C\int_{R\to 0}^{R\to\infty}F(R)f(\xi R)\frac{D(R,r)}{D(R,\xi)}dR\,d\xi\,, \tag{3.1}$$

where C is the normalizing factor and $\frac{D(R,r)}{D(R,\xi)}$ is Jacobian.

The integral (3.1) can be solved using Appendix C. If in the integral of general form (C1) we substitute R for x, -2 for α, R_1 for u_1, $\overline{R}^2/R_1$ for v_1, r_1/ξ for u_2, $\overline{r}^2/(r_1\xi)$ for v_2, δ for β, ρ for γ, we find, on the basis on (C2), the probability that ξ arrives in a range $(\xi, \xi + d\xi)$:

$$h(\xi)d\xi = C_{\xi c}\,\xi^{-3/2}\exp\left[-\frac{(\ln\xi - \ln\xi_{1c})(\ln\xi - \ln\xi_{2c})}{2(\delta^2+\rho^2)}\right]d\xi, \tag{3.2}$$

where $C_{\xi c}$ is the normalizing factor and $\sqrt{\xi_{1c}\xi_{2c}} = \frac{\overline{r}}{\overline{R}}\exp\delta^2$.

The normalized condition:

$$\int_0^1 h(\xi)d\xi = 1 \tag{3.3}$$

leads to

$$C_{\xi c} = \frac{1}{\int_0^1 \xi^{-3/2}\exp\left[-\frac{(\ln\xi - \ln\xi_{1c})(\ln\xi - \ln\xi_{2c})}{2(\delta^2+\rho^2)}\right]d\xi} \tag{3.4}$$

The integral in the denominator of (3.4) will be determined using (A3) and (A4). If we put in (A3): $x = \xi$, $p = -3/2$, $x_{1p} = \xi_{1c}$, $x_{2p} = \xi_{2c}$, $\zeta_p = \sqrt{\delta^2+\rho^2}$ we find by using (A4) the density function of *the shape parameter* ξ:

$$h(\xi) = \frac{\xi^{-3/2}\exp\left[-(\ln\xi - \ln\xi_{1c})\left(\ln\xi - \ln\frac{(\overline{r}/\overline{R})^2\exp(2\delta^2)}{\xi_{1c}}\right)\Big/\left(2(\delta^2+\rho^2)\right)\right]}{\xi_{1c}^{-1/2}\sqrt{2\pi(\delta^2+\rho^2)}\exp\left\{\frac{\left[\delta^2+\rho^2+\ln\left(\xi_{1c}^2/\left((\overline{r}/\overline{R})^2\exp(2\delta^2)\right)\right)\right]^2}{8(\delta^2+\rho^2)}\right\}\left[\phi\left(\frac{2\ln(\overline{R}/\overline{r})+\rho^2-\delta^2}{2\sqrt{\delta^2+\rho^2}}\right)+\frac{1}{2}\right]} \tag{3.5}$$

This distribution (3.5) has the similar form as one of the LG2.

The mean value of *the shape parameter* is

$$\overline{\xi} = \int_0^1 \xi\, h(\xi)d\xi. \tag{3.6}$$

The integral in (3.6) can be solved using Appendix A. By changing of variables: $x = \xi$, $p = -1/2$, $x_{1p} = \xi_{1c}$, $x_{2p} = \xi_{2c}$, $\zeta_p = \sqrt{\delta^2+\rho^2}$, $\sqrt{\xi_{1c}\xi_{2c}} = \frac{\overline{r}}{\overline{R}}\exp\delta^2$ in (A3), we find according to (A4)

$$\overline{\xi} = \frac{\overline{r}}{\overline{R}}\exp\delta^2\,\frac{-\phi\left(\frac{2\ln(\overline{r}/\overline{R})+3\delta^2+\rho^2}{2\sqrt{\delta^2+\rho^2}}\right)+\frac{1}{2}}{\phi\left(\frac{2\ln(\overline{R}/\overline{r})+\rho^2-\delta^2}{2\sqrt{\delta^2+\rho^2}}\right)+\frac{1}{2}}. \tag{3.7}$$

For the $Nd_2Fe_{14}B$ particles we obtain $\overline{\xi} = 0.64821$.

The mean value of *the shape parameter* square is:

$$\left\langle\xi^2\right\rangle = \int_0^1 \xi^2\, h(\xi)d\xi.$$

The integral in (3.8) can be solved using Appendix A, too. On making change of variables $x = \xi$, $p = 1/2$, $x_{1p} = \xi_{1c}$, $x_{2p} = \xi_{2c}$, $\zeta_p = \sqrt{\delta^2+\rho^2}$, $\sqrt{\xi_{1c}\xi_{2c}} = \frac{\overline{r}}{\overline{R}}\exp\delta^2$ in (A3), we have using (A4):

$$\left\langle\xi^2\right\rangle = \left(\frac{\overline{r}}{\overline{R}}\right)^2\exp(3\delta^2+\rho^2)\frac{-\phi\left(\frac{2\ln(\overline{r}/\overline{R})+5\delta^2+3\rho^2}{2\sqrt{\delta^2+\rho^2}}\right)+\frac{1}{2}}{\phi\left(\frac{2\ln(\overline{R}/\overline{r})+\rho^2-\delta^2}{2\sqrt{\delta^2+\rho^2}}\right)+\frac{1}{2}}. \tag{3.9}$$

For the $Nd_2Fe_{14}B$ particles $\left\langle\xi^2\right\rangle = 0.45538$. (3.10)

By using (A9), (3.7) and (3.9) we find the variance

$$\sigma_\xi^2 = \frac{\left(\frac{\overline{r}}{\overline{R}}\right)^2\exp(2\delta^2)}{\phi\left(\frac{2\ln(\overline{R}/\overline{r})+\rho^2-\delta^2}{2\sqrt{\delta^2+\rho^2}}\right)+\frac{1}{2}}\left\{\exp(\delta^2+\rho^2)\left[\frac{1}{2}-\phi\left(\frac{2\ln(\overline{r}/\overline{R})+5\delta^2+3\rho^2}{2\sqrt{\delta^2+\rho^2}}\right)\right]-\frac{\left[-\phi\left(\frac{2\ln(\overline{r}/\overline{R})+3\delta^2+\rho^2}{2\sqrt{\delta^2+\rho^2}}\right)+\frac{1}{2}\right]^2}{\phi\left(\frac{2\ln(\overline{R}/\overline{r})+\rho^2-\delta^2}{2\sqrt{\delta^2+\rho^2}}\right)+\frac{1}{2}}\right\} \tag{3.11}$$

For the $Nd_2Fe_{14}B$ particles the variance is $\sigma_\xi^2 = 0.035197$ and the standard deviation is $\sigma_\xi = 0.18761$.

If all particles have the shape of ellipse the well-known canonical equation of which is $\frac{x^2}{a^2}+\frac{y^2}{b^2}=1$, $(b \le a)$ then the longest dimension is $2a$, and the shortest dimension is $2b$. According to the aforementioned definition we can say that two particles of the elliptic shape are mutually similar if they have the same $b/a(=\xi)$ ratio. Moreover, these particles are mutually similar in mathematical meaning of the word.

The probability density distribution curve of *the shape parameter* ξ is shown in Fig. 4.

The most of the particles have shortest/longest dimension ratio around 0.6 or $3:5$. The probability density that the particle is of the circular shape is about 0.97. The probability that ξ arrives in the range

$(0.9,\ 1)$ (the particles are approximately circular) is about 11%.

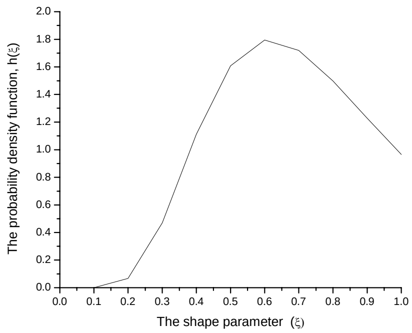

Fig. 4. The probability density distribution curve of the shape parameter ξ.

4. An approach to the generalized similarity of the particles

As foresaid, some useful properties of the sample, may be related to shape of individual particles. For example, if all particles are geometrically similar, all the subsequent treatment is simplified substantially in terms of shape. Hence, it is sometimes important to analyze similarity of the particles. The purpose of this section is development and application of a method for evaluation of the particle similarity for particular case of elliptic particles.

Consider again an assembly of n particles. Let us start from the identity

$$\sum_{i=1}^{n} R_i^2\left(t+\frac{r_i}{R_i}\right)^2=\left(\sum_{i=1}^{n} R_i^2\right)t^2+\left(2\sum_{i=1}^{n} R_i r_i\right)t+\left(\sum_{i=1}^{n} r_i^2\right), \qquad (4.1)$$

where t is any real number and R_i and r_i are the longest and shortest dimension, respectively, of i th particle. The right hand side can be rewritten in the form

$$\left(\sum_{i=1}^{n} R_i^2\right)\left(t+\frac{\sum_{i=1}^{n} R_i r_i}{\sum_{i=1}^{n} R_i^2}\right)^2+\frac{\left(\sum_{i=1}^{n} R_i^2\right)\left(\sum_{i=1}^{n} r_i^2\right)-\left(\sum_{i=1}^{n} R_i r_i\right)^2}{\sum_{i=1}^{n} R_i^2}. \qquad (4.2)$$

On dividing (4.2) by $\left(\sum_{i=1}^{n} r_i^2\right)$ and using (4.1) the following function is obtained

$$g(t)=\frac{1}{\left(\sum_{i=1}^{n} r_i^2\right)}\sum_{i=1}^{n} R_i^2\left(t+\frac{r_i}{R_i}\right)^2=\frac{\left(\sum_{i=1}^{n} R_i^2\right)}{\left(\sum_{i=1}^{n} r_i^2\right)}\left(t+\frac{\sum_{i=1}^{n} R_i r_i}{\sum_{i=1}^{n} R_i^2}\right)^2+1-\frac{\left(\sum_{i=1}^{n} R_i r_i\right)^2}{\left(\sum_{i=1}^{n} R_i^2\right)\left(\sum_{i=1}^{n} r_i^2\right)}$$

$$=\frac{\left(\sum_{i=1}^{n} R_i^2\right)}{\left(\sum_{i=1}^{n} r_i^2\right)}\left(t+\frac{\sum_{i=1}^{n} R_i r_i}{\sum_{i=1}^{n} R_i^2}\right)^2+\frac{\sum_{i=2}^{n}\left(\sum_{j=1}^{i-1}\left(R_i R_j\right)^2\left(\frac{r_i}{R_i}-\frac{r_j}{R_j}\right)^2\right)}{\left(\sum_{i=1}^{n} R_i^2\right)\left(\sum_{i=1}^{n} r_i^2\right)}. \qquad (4.3)$$

On making the substitution $t=-\frac{\sum_{i=1}^{n} R_i r_i}{\sum_{i=1}^{n} R_i^2}$ we can write:

$$\frac{1}{\left(\sum_{i=1}^{n} r_i^2\right)}\sum_{i=1}^{n} R_i^2\left(\frac{r_i}{R_i}-\frac{\sum_{i=1}^{n} R_i r_i}{\sum_{i=1}^{n} R_i^2}\right)^2=1-\frac{\left(\sum_{i=1}^{n} R_i r_i\right)^2}{\left(\sum_{i=1}^{n} R_i^2\right)\left(\sum_{i=1}^{n} r_i^2\right)}=\frac{\sum_{i=2}^{n}\left(\sum_{j=1}^{i-1}\left(R_i R_j\right)^2\left(\frac{r_i}{R_i}-\frac{r_j}{R_j}\right)^2\right)}{\left(\sum_{i=1}^{n} R_i^2\right)\left(\sum_{i=1}^{n} r_i^2\right)} \qquad (4.4)$$

Let us introduce the notation

$$\eta=\frac{\left(\sum_{i=1}^{n} R_i r_i\right)^2}{\left(\sum_{i=1}^{n} R_i^2\right)\left(\sum_{i=1}^{n} r_i^2\right)}. \qquad (4.5)$$

and by substituting into (4.4) we obtain

$$\frac{1}{\left(\sum_{i=1}^{n} r_i^2\right)}\sum_{i=1}^{n} R_i^2\left(\frac{r_i}{R_i}-\frac{\sum_{i=1}^{n} R_i r_i}{\sum_{i=1}^{n} R_i^2}\right)^2=1-\eta=\frac{\sum_{i=2}^{n}\left(\sum_{j=1}^{i-1}\left(R_i R_j\right)^2\left(\frac{r_i}{R_i}-\frac{r_j}{R_j}\right)^2\right)}{\left(\sum_{i=1}^{n} R_i^2\right)\left(\sum_{i=1}^{n} r_i^2\right)}. \qquad (4.6)$$

Since the left and right hand sides of (4.6) are the sums of squares it is clear that:

a) $1-\eta\geq 0$, i. e. $1\geq\eta>0$ (4.7)

and

b)

$$\left((\forall i)(\forall j)(i\neq j)\ \frac{r_i}{R_i}=\frac{r_j}{R_j}\right)\Leftrightarrow\left(\frac{r_i}{R_i}=\frac{\sum_{i=1}^{n} R_i r_i}{\sum_{i=1}^{n} R_i^2},\ \ i=1,2,3,\ldots,n\right)\Leftrightarrow(\eta=1) \qquad (4.8)$$

or η is equal to unity if, *and only if*, all particles have the same ξ, and

$$\xi=\frac{\sum_{i=1}^{n} R_i r_i}{\sum_{i=1}^{n} R_i^2}. \qquad (4.9)$$

Having in view a) and b) it can be concluded that if η is equal to unity all particles are mutually *generally similar* and their *shape parameter* is $\frac{\sum_{i=1}^{n} R_i r_i}{\sum_{i=1}^{n} R_i^2}$.

If we substitute $-\overline{\xi}$ for t in (4.3) we have:

$$g\left(t=-\overline{\xi}\right)=\frac{1}{\left(\sum_{i=1}^{n} r_i^2\right)}\sum_{i=1}^{n} R_i^2\left(\xi_i-\overline{\xi}\right)^2=\frac{\left(\sum_{i=1}^{n} R_i^2\right)}{\left(\sum_{i=1}^{n} r_i^2\right)}\left(\frac{\sum_{i=1}^{n} R_i r_i}{\sum_{i=1}^{n} R_i^2}-\overline{\xi}\right)^2+1-\eta, \qquad (4.10)$$

where $\xi_i = \dfrac{r_i}{R_i}$. The following inequalities are fulfilled:

$$\frac{nR_{\min}^2\sigma_\xi^2}{\left(\sum_{i=1}^n r_i^2\right)} \le \frac{1}{\left(\sum_{i=1}^n r_i^2\right)}\sum_{i=1}^n R_i^2\left(\xi_i-\bar{\xi}\right)^2 \le \frac{nR_{\max}^2\sigma_\xi^2}{\left(\sum_{i=1}^n r_i^2\right)}, \quad (4.11)$$

where $R_{\min} = \min\{R_1, R_2, \ldots R_n\}$,

$R_{\max} = \max\{R_1, R_2, \ldots R_n\}$ and $\sigma_\xi^2 = \dfrac{1}{n}\sum_{i=1}^n\left(\xi_i-\bar{\xi}\right)^2$ is the variance*.

On combining (4.10) and (4.11) it follows:

$$\frac{\sigma_\xi^2}{\frac{1}{n}\left(\sum_{i=1}^n r_i^2\right)}R_{\min}^2 \le \frac{\left(\sum_{i=1}^n R_i^2\right)}{\left(\sum_{i=1}^n r_i^2\right)}\left(\frac{\sum_{i=1}^n R_i r_i}{\sum_{i=1}^n R_i^2}-\bar{\xi}\right)^2 + 1-\eta \le \frac{\sigma_\xi^2}{\frac{1}{n}\left(\sum_{i=1}^n r_i^2\right)}R_{\max}^2 . \quad (4.12)$$

$$\frac{\sigma_\xi^2}{\langle r^2\rangle}R_{\min}^2 \le \frac{\left(\sum_{i=1}^n R_i^2\right)}{\left(\sum_{i=1}^n r_i^2\right)}\left(\frac{\sum_{i=1}^n R_i r_i}{\sum_{i=1}^n R_i^2}-\bar{\xi}\right)^2 + 1-\eta \le \frac{\sigma_\xi^2}{\langle r^2\rangle}R_{\max}^2, \quad (4.13)$$

where $\langle r^2\rangle$ is the mean value of r^2.

Hence, if the variance tends to zero the factor η will cluster more and more closely about unity, or

if $\sigma_\xi \to 0$, then $\bar{\xi} \to \dfrac{\sum_{i=1}^n R_i r_i}{\sum_{i=1}^n R_i^2}$ and $\eta \to 1$.

For the $Nd_2Fe_{14}B$ particles:

$$0.016 \le \frac{\left(\sum_{i=1}^n R_i^2\right)}{\left(\sum_{i=1}^n r_i^2\right)}\left(\frac{\sum_{i=1}^n R_i r_i}{\sum_{i=1}^n R_i^2}-\bar{\xi}\right)^2 + 1-\eta \le 0.16 . \quad (4.14)$$

If the particles are of the elliptic shape, then it can be written

$S_i = \dfrac{\pi}{4}R_i r_i$ or $R_i r_i = \dfrac{4S_i}{\pi}$. Thus,

$$\eta = \frac{\left(\frac{4}{\pi}\right)^2\left(\sum_{i=1}^n S_i\right)^2}{\left(\sum_{i=1}^n R_i^2\right)\left(\sum_{i=1}^n r_i^2\right)} = \left(\frac{4}{\pi}\right)^2\frac{\left(\bar{S}\right)^2}{\langle R^2\rangle\langle r^2\rangle}, \quad (4.15)$$

where $\langle R^2\rangle$ is the mean value of R^2.

* The variance is defined by $\sigma^2 = \sum_{i=1}^n\left(\xi_i-\bar{\xi}\right)^2 \Big/ (n-1)$. However, when n is large, the diference between using n or $(n-1)$ as divisor is small and it can be of little importance if we replace the summation by integration, later.

By putting $p = -3/2$ in (A8) we have

$$\langle R^2\rangle = \left(\bar{R}\right)^2\exp\left(\delta^2\right) \text{ and } \langle r^2\rangle = \left(\bar{r}\right)^2\exp\left(\rho^2\right). \quad (4.16)$$

On combining (4.15) and (4.16) we find

$$\eta = \left(\frac{\bar{S}}{\pi\bar{R}\bar{r}/4}\right)^2\exp\left[-\left(\delta^2+\rho^2\right)\right]. \quad (4.17)$$

For the $Nd_2Fe_{14}B$ particles: $\eta \approx 0.81$.

This approach has the advantage that the expression of the coefficient η is simpler than the expression of the standard deviation σ_ξ. The disadvantages are that the model can not be applied to nonelliptic particles and does not enable the estimation of the degree of similarity of the elliptical particles. Namely, the method could be useful for the fast interpretation of only two cases: the particles are mutually similar $(\eta = 1)$ or the particles are not mutually similar. If the particles are not mutually similar then $0 < \eta < 1$, but in this way it is not possible to determine the value of η. For the similarity degree estimation the variance of the shape parameter, σ_ξ^2 may be used.

4.1. The elliptic factor of the assembly of particles

The geometric mean value of S_i $(i = 1, 2, \ldots, n)$, under assumption that the particles are of elliptic shape, is:

$$S_g = \sqrt[n]{S_1 S_2 S_3 \ldots S_n} = \sqrt[n]{\frac{\pi}{4}R_1 r_1\frac{\pi}{4}R_2 r_2\frac{\pi}{4}R_3 r_3\ldots\frac{\pi}{4}R_n r_n} . \quad (4.1.1)$$

From (4.1.1) follows

$$S_g = \sqrt[n]{\left(\frac{\pi}{4}\right)^n R_1 R_2 R_3 \ldots R_n\, r_1 r_2 r_3 \ldots r_n} = \frac{\pi}{4}\sqrt[n]{R_1 R_2 R_3 \ldots R_n}\,\sqrt[n]{r_1 r_2 r_3 \ldots r_n} = \frac{\pi}{4}R_g r_g \quad (4.1.2)$$

where R_g is the geometric mean value of R_i $(i = 1, 2, \ldots, n)$ and r_g is the geometric mean value of r_i. $(i = 1, 2, \ldots, n)$. Then, the following relations are satisfied (Appendix B) ($p = -3/2$):

$$S_g = \bar{S}\exp\left(-w^2/2\right) \quad (4.1.3)$$

$$R_g = \bar{R}\exp\left(-\delta^2/2\right) \quad (4.1.4)$$

$$r_g = \bar{r}\exp\left(-\rho^2/2\right). \quad (4.1.5)$$

Now, we introduce parameter:

$$\nu = \frac{S_g}{\frac{\pi}{4}R_g r_g} . \quad (4.1.6)$$

Substituting (4.1.3) - (4.1.5) into (4.1.6) we find

$$\nu = \frac{\bar{S}}{\frac{\pi}{4}\bar{R}\bar{r}}\exp\frac{\delta^2+\rho^2-w^2}{2} . \quad (4.1.7)$$

It is clear that for particles of elliptic shape, ν is equal to unity. Generally, for arbitrary shapes of particles,

ν may be greater or less than unity. Having in view the bulk description of the particles, the parameter ν may be used as the parameter to measure the degree of elliptic shape of an assembly. Then we denote ν *the elliptic factor* of the assembly of particles. We also introduce „*equivalent elliptic particle*“, an imaginary particle of the elliptic shape for which the longest and shortest dimensions (axes) are equal to those of the projected particles. If ν is less than unity, the bigger particles are mostly close to a polygonal shape whose surface is smaller than surface of „*equivalent elliptic particle*“ and the smaller particles are mostly of approximate elliptic shape. If ν is greater than unity the shape of the projected particles has dominant convexity of jagged outline with regard to the outline shape of an imaginary elliptic particle for which the longest and shortest dimensions are equal to these projected particles. For the $Nd_2Fe_{14}B$ particles we find that $\nu \approx 0.96$, this being in agreement with the analyses by the microscopes and the quantitative image analyzer.

On combining (4.17) and (4.1.7) it is obtained:

$$\eta = \exp\left[w^2 - 2\left(\delta^2 + \rho^2\right)\right]. \qquad (4.1.8)$$

According to the above conclusion that the particles of elliptical shape are mutually similar for $\eta = 1$ it follows that in this case $w^2 - 2\left(\delta^2 + \rho^2\right) = 0$ or $w = \sqrt{2\left(\delta^2 + \rho^2\right)}$. From $1 \geq \eta > 0$ we have $w^2 - 2\left(\delta^2 + \rho^2\right) \leq 0$ or $w \leq \sqrt{2\left(\delta^2 + \rho^2\right)}$.

5. Conclusions

The new logarithmic distribution defined by four parameters and denoted as LG4 is proposed in this paper. One special case of the LG4 is the distribution function defined by two parameters, LG2. The mean value, as the size parameter, appeared explicitly in this distribution. The LG2 parameters are determined from a best fitting to the empirical distributions of various projected $Nd_2Fe_{14}B$ particles parameters (the longest and shortest dimensions and the surface area of the particles). The LG2 equation has been adopted as a model for shape distributions of the $Nd_2Fe_{14}B$ particles. However, the performed modelling may be useful for various applications regardless of the type of particles. *The shape parameter* of the particle is introduced and then *the generalized similarity* and *the elliptic fa*ctor of the assembly of particles are defined. Using the LG2 distribution of the longest and shortest dimensions *the shape parameter* distribution is determined. Method for the particle similarity consideration is developed. The procedure of this method is simple, easy and quick, but the method has limited application range and it can be useful for the description of elliptical particles.

Notation

Useful facts about the Poisson's integral, Error Function and Laplace's function:

Poisson's integral: $I_P = \int_0^\infty \exp\left(-u^2\right)du = \frac{\sqrt{\pi}}{2}$

The Error Function: $erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp\left(-u^2\right)du$

Laplace function: $\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_0^x \exp\left(-\frac{u^2}{2}\right)du$

Appendices

Appendix A

The probability density function of the LG4 distribution (PDFLG4) is:

$$f_p(x) = C_p x^p \exp\left[-\frac{\left(\ln x - \ln x_{1p}\right)\left(\ln x - \ln x_{2p}\right)}{2\zeta_p^2}\right], \qquad (A1)$$

where C_p is the normalizing factor. The function is normalized if the value of the integral over all possible values of x is unity, i.e. $\int_0^\infty f_p(x)dx = 1$. Hence, we have

$$C_p = \frac{1}{\int_0^\infty x^p \exp\left[-\frac{\left(\ln x - \ln x_{1p}\right)\left(\ln x - \ln x_{2p}\right)}{2\zeta_p^2}\right]dx} = \frac{1}{I_A}\cdot \qquad (A2)$$

In order to obtain the normalizing factor we have to determine the integral

$$I_A^{ind} = \int x^p \exp\left[-\frac{\left(\ln x - \ln x_{1p}\right)\left(\ln x - \ln x_{2p}\right)}{2\zeta_p^2}\right]dx. \qquad (A3)$$

By making the change of variables $\ln x = t$ we have

$$I_A^{ind} = x_{1p}^{p+1}\zeta_p\sqrt{2\pi}\,\exp\left\{\frac{\left[2(p+1)\zeta_p^2 - \ln\left(x_{1p}/x_{2p}\right)\right]^2}{8\zeta_p^2}\right\}\,\phi\left(\frac{\ln\left(x/\sqrt{x_{1p}x_{2p}}\right) - (p+1)\zeta_p^2}{\zeta_p}\right) \qquad (A4)$$

Then

$$I_A = x_{1p}^{p+1}\zeta_p\sqrt{2\pi}\,\exp\left\{\frac{\left[2(p+1)\zeta_p^2 - \ln\left(x_{1p}/x_{2p}\right)\right]^2}{8\zeta_p^2}\right\}. \qquad (A5)$$

By using (A1), (A2) and (A5) we obtain the PDFLG4:

$$f_p(x) = \frac{x^p \exp\left[-\frac{\left(\ln x - \ln x_{1p}\right)\left(\ln x - \ln x_{2p}\right)}{2\zeta_p^2}\right]}{x_{1p}^{p+1}\zeta_p\sqrt{2\pi}\,\exp\left\{\frac{\left[2(p+1)\zeta_p^2 - \ln\left(x_{1p}/x_{2p}\right)\right]^2}{8\zeta_p^2}\right\}} \qquad (A6)$$

By using (A3) and (A4) it can be found that the mean value of the PDFLG4 is

$$\bar{x}_p = \int_0^\infty x f_p(x) dx = \frac{\int_0^\infty x^{p+1} \exp\left[-\frac{(\ln x - \ln x_{1p})(\ln x - \ln x_{2p})}{2\zeta_p^2}\right] dx}{x_{1p}^{p+1} \zeta_p \sqrt{2\pi} \exp\left\{\frac{\left[2(p+1)\zeta_p^2 - \ln(x_{1p}/x_{2p})\right]^2}{8\zeta_p^2}\right\}} = \sqrt{x_{1p} x_{2p}} \exp\left(\frac{(2p+3)\zeta_p^2}{2}\right) \quad \text{(A7)}$$

and the mean value of x^2 is

$$\left\langle x^2 \right\rangle_p = \int_0^\infty x^2 f_p(x) dx = x_{1p} x_{2p} \exp\left[2(p+2)\zeta_p^2\right]. \quad \text{(A8)}$$

The variance of the PDFLG4 is

$$\sigma_p^2 = \left\langle \left(x - \bar{x}_p\right)^2 \right\rangle = \int_0^\infty \left(x - \bar{x}_p\right)^2 f_p(x) dx = \int_0^\infty \left(x^2 - 2x\bar{x}_p + \bar{x}_p^2\right) f_p(x) \; dx = \left\langle x^2 \right\rangle_p - \bar{x}_p^2 \quad \text{(A9)}$$

Substituting (A7) and (A8) into (A9) we find the variance

$$\sigma_p^2 = x_{1p} x_{2p} \exp\left[(2p+3)\zeta_p^2\right] \left[\exp\left(\zeta_p^2\right) - 1\right] \quad \text{(A10)}$$

and the standard deviation

$$\sigma_p = \sqrt{x_{1p} x_{2p}} \exp\left(\frac{2p+3}{2}\zeta_p^2\right) \sqrt{\exp\left(\zeta_p^2\right) - 1}. \quad \text{(A11)}$$

Appendix B

Let $x_i \;\; (i = 1, 2, ..., n)$ be the value of some parameter of ith particle. The geometric mean value of the values x_i is:

$$x_g = \exp\left(\int_0^\infty (\ln x) \; f_p(x) dx\right). \quad \text{(B1)}$$

By using the change of variable: $t = \ln x$ we have

$$x_g = \exp\left(\overline{\ln x}\right) = \sqrt{x_{1p} x_{2p}} \exp\left[(p+1)\zeta_p^2\right]. \quad \text{(B2)}$$

Appendix C

Let us solve the following integral:

$$I_C = \int x^\alpha \exp\left[-\frac{(\ln x - \ln u_1)(\ln x - \ln v_1)}{2\beta^2}\right] \exp\left[-\frac{(\ln x - \ln u_2)(\ln x - \ln v_2)}{2\gamma^2}\right] dx \quad \text{(C1)}$$

By making the change of variable: $t = \ln x$ and after some transformations similar (but more complicated) to those in Appendix A we have the result:

$$I_C = \sqrt{\frac{2\pi}{\left(\frac{1}{\beta^2} + \frac{1}{\gamma^2}\right)}} \exp\left[\frac{\left(2(\alpha+1)\beta\gamma + \frac{\gamma}{\beta}\ln(u_1 v_1) + \frac{\beta}{\gamma}\ln(u_2 v_2)\right)^2}{8\left(\beta^2 + \gamma^2\right)} - \frac{1}{2}\left(\frac{(\ln u_1)(\ln v_1)}{\beta^2} + \frac{(\ln u_2)(\ln v_2)}{\gamma^2}\right)\right]$$

$$\times \; \Phi\left[\frac{\sqrt{\beta^2 + \gamma^2}}{\beta\gamma} \;\; \ln x - \frac{2(\alpha+1)\beta\gamma + \frac{\gamma}{\beta}\ln(u_1 v_1) + \frac{\beta}{\gamma}\ln(u_2 v_2)}{2\sqrt{\left(\beta^2 + \gamma^2\right)}}\right] \quad \text{(C2)}$$

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