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THE EFFECT OF THE SHAPE FUNCTION ON
SMALL-ANGLE SCATTERING ANALYSIS BY
THE MAXIMUM ENTROPY METHOD

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Abstract

Analysis of small-angle scattering data to obtain a particle size distribution is dependent upon the shape function used to model the scattering. Using a maximum entropy analysis of small-angle scattering data, the effect of shape function selection on the obtained size distribution is demonstrated using three different shape functions to describe the same scattering data from each of two alloys. The alloys have been revealed by electron microscopy to contain a distribution of randomly oriented and mainly non-interacting, irregular, ellipsoidal precipitates. Comparison is made between the different forms of the shape function. The effect of an incident wavelength distribution is also shown. The importance of testing appropriate shape functions and validating these against other microstructural studies is discussed.

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Analysis of small-angle scattering data to obtain a particle size distribution is dependent upon the shape function used to model the scattering. Using a maximum entropy analysis of small-angle scattering data, the effect of shape function selection on the obtained size distribution is demonstrated using three different shape functions to describe the same scattering data from each of two alloys. The alloys have been revealed by electron microscopy to contain a distribution of randomly oriented and mainly non-interacting, irregular, ellipsoidal precipitates. Comparison is made between the different forms of the shape function. The effect of an incident wavelength distribution is also shown. The importance of testing appropriate shape functions and validating these against other microstructural studies is discussed.

I. INTRODUCTION

Diffraction measured at small-angles is often due to compositional inhomogeneities that extend over the length scale of nanometers to micrometers. Should these inhomogeneities or *scatterers* adhere to certain basic assumptions of morphology, such as those outlined by Shull and Roess (Roess & Shull, 1947, Shull & Roess, 1947), the small-angle scattering may be interpreted as evidence of an underlying size distribution of the scatterers. Approximation of the underlying size distribution proceeds by fitting appropriate distribution parameters to the measured intensity data. One such method of obtaining a size distribution from small-angle scattering data is the maximum entropy method, increasingly known as *MaxEnt* (Potton, Daniell, & Rainford, 1988).

A common assumption about the morphology is that the scatterers all have the same definite shape, although certain characteristic dimensions may differ between scatterers. For example, in the case of cylindrically-shaped scatterers, the ratio between the cylinder length and diameter might be assumed to remain constant, regardless of the cylinder diameter. Other frequently-made assumptions are that interference between the inhomogeneities is negligible, that the composition gradient is sharp at the boundary of each scatterer so that the scatterers are well-defined, that the composition of each scatterer is constant within its boundary, and that the scatterers are randomly oriented. Additionally, it is often assumed that the incident radiation is monochromatic and the sample is sufficiently thin so that multiple scattering can be neglected.

All the assumptions about the morphology of the scatterers are described, either implicitly or explicitly, through the use of a *shape function*. In some cases, the choice of an appropriate shape function may not be straightforward. Through changes in the distribution parameters, different shape functions may be used to arrive at the same

calculated intensity profile. Further constraint in shape function selection is provided by comparison with other experimental or theoretical evidence. Such evidence might include examination of the samples by transmission electron microscopy (TEM) or atom probe field ion microscopy (AP/FIM), or might result from consideration of the constraints placed by appropriate compositional or thermodynamic boundary conditions on the MaxEnt results from particularly well-characterized sample material (Allen, Gavillet, & Weertman, 1992). Information about instrumental collimation may also be included in the definition of the shape function (Potton, Daniell, & Rainford, 1988).

Entropy maximization produces the most uniform approximation to the underlying size distribution that is consistent with the experimental intensity data within the limits of experimental uncertainty. An advantage of MaxEnt is that an assumption about the general form of the size distribution (*e.g.*, Gaussian, unimodal, etc.) need not be made nor is it necessary to extrapolate the intensity data beyond the measured range.

It has been observed that size distributions obtained by a maximization of their configurational entropy show minor high frequency structure. This effect is demonstrated in Fig. 1, which shows two size distributions. The solid line indicates a hypothetical distribution of spherical scatterers, constructed as the sum of two log-normal distribution functions. Such distributions are typical of the distributions obtained from a MaxEnt analysis of small-angle neutron scattering (SANS) data from ultrahigh-strength steels. From this hypothetical distribution, small-angle scattering intensity data were calculated, including a typical background and pseudo-random noise. The open circles are the MaxEnt approximation of the size distribution giving rise to the simulated intensity data. The principle features of the initial size distribution are recovered but an additional, minor higher-frequency component has been

introduced into the distribution.

The source of these oscillations has been attributed (Allen, Gavillet, & Weertman, 1992) to the presence of trigonometric terms in the shape functions employed to describe the scattering. In one of the shape functions to be considered, a rational polynomial was derived (Allen, Gavillet, & Weertman, 1992) to approximate the appropriate shape functions, thereby eliminating the minor oscillations from the size distributions.

In this paper, we seek to demonstrate how consideration of different shape functions (hence different assumed scatterer morphologies) affects the MaxEnt size distributions obtained from small-angle scattering studies of a real, complex alloy system.

II. SHAPE FUNCTIONS

A volume fraction size distribution, $f(r)$, can be determined from the small-angle scattering intensity (see for example: Jemian, Weertman, Long, & Spal, 1990) by solving

$$I(h) = |\Delta\rho|^2 \int_0^\infty S(h,r)V(r)f(r)dr \quad (1)$$

using a MaxEnt method (Potton, Daniell, & Rainford, 1988). Here, $h = (4\pi/\lambda_0) \sin \theta$, where 2θ is the scattering angle, λ_0 is the wavelength of the incident monochromatic radiation, r is the characteristic linear dimension of the scatterer, $S(h,r)$ is defined as the *shape function* of the scatterers, $V(r)$ is the volume of a scatterer of dimension r , and $f(r)dr$ is the volume fraction of scatterers of size between r and $r + dr$. The scattering contrast, $|\Delta\rho|^2$, is considered independent of the size of the scatterers, but must of course be evaluated precisely to give an accurate absolute scale for the volume fraction size distribution of the scatterers.

If polychromatic radiation is used, the shape function broadens by

$$\tilde{S}(h, r) = \int_0^\infty P_\lambda(\lambda) S\left(\frac{h\lambda_0}{\lambda}, r\right) d\lambda, \quad (2)$$

where $P_\lambda(\lambda)$ is the probability distribution of wavelengths. Assuming that the incident wavelength distribution is triangular with peak at λ_0 and full-width at half-maximum $\Delta\lambda$,

$$P_\lambda(\lambda) = 1 - \left| \frac{\lambda - \lambda_0}{\Delta\lambda} \right|, \quad (3)$$

for $\lambda_0 - \Delta\lambda \leq \lambda \leq \lambda_0 + \Delta\lambda$ and zero elsewhere.

For randomly-oriented, non-interacting, spherical scatterers of diameter $2r$, we can write:

$$S_s(h, r) = \frac{9}{(hr)^6} [\sin(hr) - (hr) \cos(hr)]^2. \quad (4)$$

The subscript s is used to denote the type of shape function.

Shull and Roess (Roess & Shull, 1947, Shull & Roess, 1947) have shown that for randomly-oriented, non-interacting, regular ellipsoidal scatterers with a fixed aspect ratio, β , and major axes $2r \times 2r \times 2r\beta$,

$$S_e(h, r) = \int_0^1 S_s \left[hr \sqrt{1 + x^2(\beta^2 - 1)} \right] dx. \quad (5)$$

The integration over x accounts for all orientations of the scatterer. This analytical function is exact for regular ellipsoids with any single β over the entire range of aspect ratios: $0 < \beta < \infty$. The ellipsoid shape function of Shull and Roess, both with and without wavelength smearing, forms the basis of two of the three shape functions used in the comparison study below.

The shape function utilized by one of us (AJA) in previous work (Allen, Gavillet, & Weertman, 1992) is an attempt to describe the scattering in the presence of a broad distribution of incident wavelengths from randomly-oriented, non-interacting, irregular, globular-shaped scatterers with a moderate, representative aspect ratio, β , in the range $0.3 < \beta < 3.5$:

$$S_g(h, r) = \frac{1}{1 + \frac{1}{15}h^2r^2(2 + \beta^2) + \frac{2\beta}{9\chi}h^4r^4}. \quad (6)$$

For the application considered in the present paper ($\beta \geq 1$), so

$$\chi \equiv \frac{1 + \frac{\beta^2}{\sqrt{\beta^2-1}} \sin^{-1} \left(\frac{\sqrt{\beta^2-1}}{\beta} \right)}{2\beta}. \quad (7)$$

The shape function S_g has the limiting behavior for a single particle of given size:

$$\lim_{hr \rightarrow 0} S_g(h, r) \simeq \exp \left[-\frac{1}{15}h^2r^2(2 + \beta^2) \right] \quad (8)$$

and

$$\lim_{hr \rightarrow \infty} S_g(h, r) \simeq \frac{9\chi}{2\beta}(hr)^{-4} \quad (9)$$

which are the correct Guinier and Porod laws (Roess & Shull, 1947, Shull & Roess, 1947), respectively, for an ellipsoid with a fixed aspect ratio, β , and major axes $2r \times 2r \times 2r\beta$. S_g is intended to be applied directly when the wavelength-smearing effects, together with those due to any disordered aspects of the sample microstructure, are sufficient to remove the Bessel function oscillations associated with $\tilde{S}_e$.

III. EXPERIMENTAL

Compositions of the two steel samples investigated are given in Table I while details of their preparation are provided elsewhere (Montgomery, 1990). Analyses of TEM micrographs (Lee & Allen, 1991) and X-ray diffraction $\theta - 2\theta$ scans (Jemian, 1992) have shown that the scatterers in alloy SRG2 aged 10 h at 510° C are rod-shaped M_2C ($M = Mo$ and Fe). In alloy AF1410 aged 10 h at 510° C, the scatterers are irregular, ellipsoidal or cylindrical, rod-shaped M_2C ($M = Cr, Mo, \text{ and } Fe$), somewhat larger precipitates of M_3C ($M = Fe, Co, \text{ and } Ni$), and precipitated austenite (Jemian, 1992) of approximate spheroidal shape. Precipitated austenite is not observed in SRG2 due to the lower Ni content. The martensitic matrix of each sample

is ferromagnetic but M_2C and austenite are each paramagnetic. Thus, both M_2C and austenite scatter as magnetic voids in the ferromagnetic matrix. The situation for M_3C is more complicated because it is ferromagnetic; there is a magnetic scattering contrast between M_3C and the matrix. However, in both alloy systems, the M_2C population is discernible as a separate size distribution at smaller length scales than the other features. The small angle scattering from M_2C precipitates, which we wish to characterize using the MaxEnt technique, is expected to lie within the measured range of scattering vectors, h . From the alloy composition, magnetic scattering lengths and knowledge of strain in the ferromagnetic matrix adjacent to the M_2C precipitates, $|\Delta\rho|^2 = 1.72 \times 10^{29} \text{ m}^{-4}$ for M_2C in alloy AF1410 (Allen, Gavillet, & Weertman, 1992) and $|\Delta\rho|^2 = 2.0 \times 10^{29} \text{ m}^{-4}$ for M_2C in alloy SRG2. (These magnetic contrasts reflect an adjustment to account for the $\pm 15^\circ$ sector averaging of the intensity data described below.) Because the matrix strain about the other precipitates is much lower, the contrast of the austenite is slightly higher than that of the M_2C by a few percent.

Small-angle neutron scattering experiments were conducted at the Cold Neutron Research Facility at the National Institute of Standards and Technology, Gaithersburg, MD. A helical velocity selector was used to select a triangular incident wavelength distribution, as described above, where $\lambda_0 = 8.5 \text{ \AA}$ and $\Delta\lambda/\lambda_0 = 0.25$. Scattered intensity was registered on a two-dimensional area detector. Sample-to-detector distances of 2.0 m and 3.6 m were used on both samples to cover a range of scattering vectors, h . For sample AF1410, the h range covered was 0.0165 to 0.104 $\text{\AA}^{-1}$ while for sample SRG2, the maximum h was increased to 0.187 $\text{\AA}^{-1}$ by offsetting the detector.

In the experiment, each sample was subjected to a saturation magnetic field of 1.2 T directed perpendicular to the direction of the incident radiation. The saturation magnetic field was used to remove the magnetic refraction broadening of the neutron

beam within the unmagnetized material. The broadening arises from the abrupt changes in the relative orientation of the neutron magnetic moment and the domain magnetization as a neutron traverses successive domain boundaries. For a magnetized sample, magnetic scattering vanishes when the scattering vector is parallel to the applied magnetic field. A contour plot of the scattered intensity on the two-dimensional detector shows an hourglass shape with the strongest scattering being observed perpendicular to the direction of the applied magnetic field. The additional scattering is due to interactions between the neutron magnetic moment and the ferromagnetization moment. After averaging intensity data on the area detector within 15° of each of these two directions, the pure magnetic scattering was obtained by subtracting the horizontal sector average from the vertical sector average and is shown after flat background subtraction in Fig. 2a.

The shapes of the two scattering curves are different. The magnetic SANS from alloy SRG2 has much lower intensity at small h than does that from alloy AF1410. This is indicative of the presence of more scatterers of large dimension in AF1410. Also, the SANS from SRG2 exhibits an inflection point that is not evident in the SANS from AF1410. Porod plots are shown in Fig. 2b. The AF1410 SANS data is shown to just reach the expected Porod plateau where $h^4 I$ is constant. SRG2 does not show evidence of a Porod region. This will be discussed below. Guinier plots of the data are not given. Due to the broad size distributions underlying the SANS from each sample, no region of the SANS curves plotted as $\log I$ vs. h^2 displays the linear characteristic of a Guinier region.

IV. DISCUSSION

The shape functions to be discussed are S_e , defined in Eq. (5), $\tilde{S}_e$, defined in Eq.s (2) and (5), and S_g , defined in Eq. (6). These functions, with $\beta = 2.5$, are

presented in Figs 3 and 4. At low hr , all functions approach unity while at high hr , the functions adhere closely to a power law with an exponent of -4. Differences are observed in the transition region from Guinier to Porod behavior: $0.9 \leq hr \leq 3$. The shape functions for S_e and $\tilde{S}_e$ undergo the transition at higher hr than does S_g . An implication of the difference in the location of the transition region in the shape functions is that a characteristic size, such as the mean diameter or the most probable diameter, obtained using S_g , may be different from the characteristic size obtained using either S_e or $\tilde{S}_e$. The integrated scattering, $\int h^2 S(h) dh$, (and hence the determined volume fractions of scatterers) will also be different. Indeed, depending on the value of β , the apparent Guinier radius can be larger for S_g than for either S_e or $\tilde{S}_e$, perhaps because S_g is more appropriate for a cylindrically-shaped particle than for an ellipsoid. However, as revealed in Fig. 4a, the slope of the curve for S_g is greater than that for the two other functions, consistent with the assumption that S_g is applicable to a more cylindrical, irregular particle shape than the ideal, regular ellipsoids considered by Shull and Roess.

Plotted in Figs 5 and 6 are the volume fraction size distributions for the two steel samples, where $D = 2r$, determined by a maximum entropy method using the shape functions S_e , $\tilde{S}_e$, and S_g . A summary of these distributions is given in Table II. Shown in Figs 7 and 8 are the SANS data and the MaxEnt solutions using the S_e , $\tilde{S}_e$, and S_g shape functions. Differences between the scattered intensities reconstructed using the three shape functions are well within the experimental errors.

The general shapes of the size distributions of Figs 5 and 6 are very different. A unimodal size distribution is indicated for alloy SRG2 while the size distribution for alloy AF1410 is polymodal. This result is obtained by each of the shape functions used. The size distributions determined are those of maximum configurational entropy necessary to reconstruct the measured SANS within the limits of experimental error.

Thus, the difference in the general shape of the obtained size distributions between the two samples is due to differences between the two samples themselves and not in the analytical technique or the shape functions employed.

Referring to the figures, at both small and large hr regimes (Guinier and Porod regimes, respectively), the shape functions are in good agreement with the scattered intensities. Comparing S_e with $\tilde{S}_e$, the wavelength-smearing has little effect on the determined size distribution, smoothing it slightly and shifting it to slightly larger size. The size distribution determined using S_g indicates a slightly smaller size for the M₂C scatterers in AF141C than do either of the shape functions S_e or $\tilde{S}_e$. This difference is more pronounced for the SRG2 sample. For the AF1410 sample, $h_{\max}\bar{r} \sim 2.8$ where $h_{\max}$ is the maximum h obtained in the experiment and $2\bar{r} = \bar{D}$ from the fit of a Gaussian to the M₂C peak of the size distribution, given in Table II. For the SRG2 sample, $h_{\max}\bar{r} \sim 1.9$. Even though the selected h range of the SANS data is smaller for the AF1410 sample than for the SRG2 sample, the AF1410 SANS data extend into the Porod regime (see Fig. 2b) of the M₂C scatterers due to the larger $\bar{r}$ of the underlying size distribution. Discrepancies in $\bar{r}$ obtained with the different shape functions may be associated with the fact that the SRG2 SANS data do not extend into the Porod scattering regime for the small $\bar{r}$ in this alloy as does the AF1410 SANS data. Hence, the differences in the shape functions in the intermediate hr regime discussed above will be more marked for SRG2. In AF1410, the discrepancies are smaller because the SANS data extend further into the Porod regime (where the different shape functions agree) for these larger scattering particles.

The area under the volume fraction size distributions is the volume fraction of scatterers. It is apparent that the use of S_g as a shape function results in a higher indicated volume fraction than does either S_e or $\tilde{S}_e$. This is easily explained by an examination of Fig. 3. S_g has a lower value in the transition region than do either S_e

or $\tilde{S}_e$, evidence that S_g has a reduced integral intensity under the scattering curve. Thus, for the globule shape function to arrive at the same magnitude of scattering intensity, the magnitude of the resultant size distribution must be increased.

Given the differences in resultant size distributions and volume fractions, it is important to determine the appropriate scattering shape function to use. For a well-defined system of non-interacting, regular ellipsoids, the above arguments point to use of $\tilde{S}_e$ where the double numerical integration is carried out to average over all orientations of the ellipsoids and over the incident wavelength spectrum. However, it should be noted that $\tilde{S}_e$ is strictly valid for distributions in which β is constant for all scatterers. Deviations from this constraint will lead to imprecision in the assessment of the scattering particle volume, integrated scattering intensity, and the characteristic size. Therefore, it is important to determine the appropriate representative value of β , weighted for the type of size distribution required (number density, volume fraction, etc).

For a complex and variable morphology such as occurs in the ultra-high strength alloys discussed here, the choice between $\tilde{S}_e$ and S_g is more difficult. $\tilde{S}_e$ certainly represents one limiting case: well-defined, regular, ellipsoids with a narrow distribution of aspect ratios and with sharply defined boundaries with the matrix phase. In these alloys, however, it is known that these assumptions leading to a choice of $\tilde{S}_e$ do not strictly apply. The M_2C have been observed to have a range of aspect ratios and considerable deviations from regular ellipsoidal shape (Montgomery, 1990, Lee & Allen, 1991). Also, complex concentration gradients exist in the ferromagnetic matrix adjacent to the M_2C .

For a nominally-defined ellipsoidal scatterer (major axes: $D \times D \times \beta D$), geometric deviations from a true ellipsoidal shape will increase the surface-to-volume ratio of the particles, and hence reduce the relative central (Guinier) scattering intensity,

compared to the Porod scattering in the tails. Concentration gradients will usually act to reduce the scattering contrast from the value assumed, causing the overall integrated intensity per particle to decline. On the other hand, a more cylindrical shape will result in a larger apparent Guinier radius for a given minor diameter. All these effects, together with any loss in particle symmetry which may arise from the asymmetric strain fields found at dislocation intersections, which are prevalent nucleation sites (Montgomery, 1990, Lee & Allen, 1991), will result in a reduction in the amplitude of the Bessel function oscillations associated with $\tilde{S}_e$. (It must be remembered that such oscillations arise mathematically from the solution of a modified wave equation at a sharp interface assumed to have ellipsoidal symmetry.) When deviations from regular ellipsoid particle geometry are also taken into account, the best choice of shape function may move away from $\tilde{S}_e$ and towards S_g .

In dealing with a complex multi-component microstructure, it can be difficult to evaluate all the factors which affect the basis for such choices. Experimental verification and validation of the size distribution analysis against other analytical and theoretical evidence becomes essential. The requirement for experimental validation becomes even stronger if a background scattering component must be subtracted. SANS analysis using the MaxEnt technique is particularly sensitive to the background subtraction. Determination of the background can be imprecise for systems in which there is a substantial migration of atomic species within the scope of the study such as during the course of the aging of precipitates in ultra-high strength steel alloys.

For the studies on AF1410 alloy (Allen, Gavillet, & Weertman, 1992), extensive calibration and validation of the size distribution results based on Eq. (6) have been made using information obtained from electron microscopy, AP/FIM, thermodynamic calculations, and mechanical properties at aging times for which such comparison information is available. Where such independent validation is possible, it has been

found that the use of the S_g shape function, with appropriately-chosen representative aspect ratios, provides valid volume fraction and particle size distribution information for the M_2C precipitates (despite the complications discussed above and the presence of larger features). With this shape function, the MaxEnt technique has been utilized to explore earlier aging times, to determine the initial nucleation size, and to observe the aging time dependence of the nucleation and coarsening phenomena of M_2C under extreme supersaturation conditions such as described by (Langer & Schwartz, 1980). The SANS results have indicated where further AP/FIM, TEM, and other diagnostic studies should be concentrated. In those cases where such studies have been performed, measurements have confirmed the SANS predictions, including confirmation of a larger initial M_2C nucleation size than previously expected (Lee & Allen, 1991).

For the SRG2 and related alloys, much of the calibration and validation work remains incomplete. However, the more controlled microstructure, reduced presence of larger scattering features, and simpler atomic composition suggest that the shape function based on S_e may be more appropriate in this case. Given the measured mean diameter of M_2C particles, additional SANS measurements may be needed to extend the scattering vector range further out into the Porod scattering region and to better quantify the background.

V. CONCLUSIONS

Three shape functions describing the small-angle scattering from randomly-oriented, non-interacting, ellipsoidal or globular scatterers of moderate aspect ratio have been compared by the analysis of experimental SANS data from two different samples of ultra-high strength steel alloys. The shape functions presented here can be used to obtain size distributions that can themselves be used to reconstruct the scattering data to within the limits of experimental error. Differences in the mean

size and total volume fraction of the distributions are attributable to differences in the transition region in the shape functions between low and high hr . These differences may have a dominant effect if the accessible h range does not fully extend into the high hr Porod regime. Conservation of the integrated scattering, $\int h^2 S(h) dh$, for the particle morphology studied is also important to estimate the volume fraction of scatterers, even if such integrals do not approach their theoretical values with the measurable hr range.

Although the general character of the size distributions (*e.g.*, unimodal *vs.* poly-modal) are shown to be independent of the shape function used, both the characteristic size and amount obtained from an analysis of SANS using the globule shape function, S_g , differ from those values obtained using the wavelength-smear, ellipsoid shape function, $\tilde{S}_e$, of Shull and Roess. Clearly, the latter should be used when the underlying assumptions (single aspect ratio, non-interacting, randomly-oriented, regular ellipsoids) remain valid. For studies on more complicated systems, for example, a statistically-representative study of the nucleation and growth kinetics of carbide precipitation in ultra-high strength steels, the choice of shape function can only be confirmed after extensive comparisons with other diagnostic techniques. It is only then that maximum entropy size distribution analysis can be fully applied in small angle scattering studies to probe microstructural information not obtainable by other methods.

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TABLES

TABLE I. Compositions of ultra-high strength steel samples (weight percent).

alloy	C	Cr	Fe	Co	Ni	Mo
AF1410	0.16	2.10	bal.	14.25	10.15	1.05
SRG2	0.24	0.06	bal.	15.99	4.96	4.03

TABLE II. Summary of MaxEnt-derived size distributions. Results are derived from both the entire distribution and from a fit of a Gaussian to the M_2C peak in the distributions.

	whole distribution				fit of Gaussian to M_2C peak		
	f_V^a	D_{mp} , Å	$\bar{D}$, Å	σ , Å	f_V	$\bar{D}$, Å	σ , Å
sample: AF1410							
S_e	.033	55.9	121	74	.012	54.7	10.0
$\tilde{S}_e$	.032	55.9	123	76	.012	55.0	10.7
S_g	.055	48.6	129	92	.022	50.5	8.7
sample: SRG2							
S_e	.027	20.4	19.9	2.6	.027	19.9	2.6
$\tilde{S}_e$	.028	20.4	26.9	2.3	.026	20.1	2.7
S_g	.058	14.7	14.5	2.4	.054	14.5	2.4

^aThe parameters are defined as follows:

$f_V = \int f(D) dD$: volume fraction

D_{mp} : most probable diameter (mode of size distribution)

$\bar{D}$: mean diameter ($= 2\bar{r}$ in text)

σ : distribution half-width

FIGURES

FIG. 1. Example volume fraction size distributions, $f(D)$, of spherical scatterers obtained from a MaxEnt analysis of simulated SANS data from a hypothetical size distribution. (—) initial, hypothetical distribution, (o) MaxEnt approximation. Here, $D = 2r$.

FIG. 2. Magnetic scattering component of the measured small-angle neutron scattering from the two steel samples. [a] $\log I$ vs. $\log h$ axes. [a] Porod plot. Vertical lines are the estimated standard deviations of the data points calculated from the counting statistics.

FIG. 3. Different shape functions used to describe the scattering from randomly-oriented, non-interacting ellipsoids with major axes $2r \times 2r \times 2r\beta$ where $\beta = 2.5$. For the wavelength-smearing, a triangular incident wavelength distribution was assumed with $\Delta\lambda/\lambda_0 = 0.25$.

FIG. 4. Plots of the limiting forms of S_e , $\tilde{S}_e$, and S_g . [a] Guinier region at low hr . [b] Porod region at high hr .

FIG. 5. Volume fraction size distribution, $f(D)$, of rod-shaped M_2C scatterers in ultra-high strength steel alloy SRG2 aged 10 h at 510° C. The aspect ratio, β , of the scatterers was assumed to be 3.7 after examination of TEM micrographs. The plot legend shows the correspondence between the indicated curve and the shape function used for the MaxEnt analysis.

FIG. 6. Volume fraction size distribution, $f(D)$, of rod-shaped M_2C and precipitated austenite scatterers in ultra-high strength steel alloy AF1410 solution heat treated for one hour at 830° C and aged 10 h at 510° C. The aspect ratio, β , of the scatterers was assumed to be 2.9 after examination of the M_2C precipitation observed in TEM micrographs. The plot legend shows the correspondence between the indicated curve and the shape function used for the MaxEnt analysis.

FIG. 7. Comparison of MaxEnt fits to SANS data from ultra-high strength steel alloy SRG2 aged 10 h at 510° C. The plot legend shows the correspondence between the indicated curve and the shape function used for the MaxEnt analysis.

FIG. 8. Comparison of MaxEnt fits to SANS data from ultra-high strength steel alloy AF1410, solution heat treated for one hour at 830° C and aged 10 h at 510° C. The plot legend shows the correspondence between the indicated curve and the shape function used for the MaxEnt analysis.

FIG.1

Fig. 2a

Fig. 3

FIG. 4a

Fig. 46

Fig. 5

FIG. 6

Fig. 7

Fig. 8

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