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The Application of Laser Beam Diffraction and Scattering Methods in the Measurement of Shape and Determination of Material Parameters

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Lasers can be used for many applications including determination of size, in addition to the theory of diffraction and material dispersion phenomena. In this paper we calculated the corrections in angular intensity for the Gaussian and uniform particle distributions, the scattering intensity on cylindrical objects. We also evaluated the necessary mathematical summations. In addition, we analyse and simulated the special positions of detectors using laser Doppler anemometric (LDA) methods, which can be used to determine the particle diameter. The dispersion measurements for actual fibres are given at the end. The geometric and material parameters of these fibres were taken before the evaluation of the angular scattering intensity.

Keywords: laser, diffraction, scattering, fibres, sensors, convergence, LDA

1 INTRODUCTION

Optical methods, employed in many research fields, are especially useful in dynamic processes. The techniques with a high degree of coherency are particularly significant. In addition to improving conventional interferometers they provide new methods of measuring not possible with other optical sources [1–3]. The development of lasers in the atto-second range and the ultimate, optical data acquisition techniques, enable measurement not only of such short pulses but at the frontier in a discussion on fundamental physical laws.

Some results of our calculations of angular intensities or angular correction factors based on fundamental theory are presented for spherical and cylindrical geometries. For the cylindrical geometry, the chosen data for calculation were taken from commercial fibre types. We measured on them dispersion characteristics which are not usually included in scattering theory. Knowing that fibre sizing can be carried out by laser devices, we wanted to show dispersion characteristics which could "blur" the diffraction figures. Considering that particle size determination is our main emphasis in this paper, we also calculated the positions of photo-detectors, which could provide the radius of scattering particle. We remind readers that holographic measurements, in the determination of size, is possible by scattering from objects, but is rarely done [4].

The aim of this paper is to point out several different problems in laser scattering (integral scattering on spherical particles, scattering on multi-layer cylindrical geometrical structures etc) and to propose the appropriate theoretical models. The applicability of this model to particular cases and it comparison with other models will be studied elsewhere.

Different aspects of light scattering phenomena, common to all experimental and numerical analysis, considered in this work, could be of interest to others. The approach presented and the measurement of for example, the diffraction integral, summation of mathematical series, could be linked to a laser application in experimental techniques for the determination of the size of a particle [1–35].

2 SCATTERING APPROACH

Integral scattering

Recently, there has been an increase in interest in light scattering by anisotropic and multi-layer material objects of various geometrical shapes, for both practical and theoretical reasons. Such an analysis enables us to determine size of the various particles – powders, droplets, macromolecules, micelles, emulsions [5–9] as well as information on particle dynamics. Starting from the expression $I(d, \theta)$ for light scattering intensity and including the particle size distribution, one can obtain a method for particle sizing by laser techniques [10, 16, 17]. Modelling this type of scattering is very complex. It includes the single particle scattering and the extension to model a large number of scattering centres or alternatively, one can start with collective modelling. The size of the scattering object, the wave vector as well as the index of refraction of the particle and the environment are of great importance in order to compare two models with two different approximations and to find the incoherency between them.

In this paper, we investigate the scattering of spherical and cylindrical particles. We start with an equation, which describes single particle scattering, and using the particle size distribution as an input parameter. We expand it to include a large number of scattering centres. Gaussian and uniform distributions are applied. The results are given as functions of the scattering angle, where at a specific scattering angle the characteristic particle size can be obtained.

Here, we follow the approach from Refs. [10, 18], where the angular distribution of the scattered light intensity is given by:

$$I(\theta) = cAL \int_0^\infty i(\alpha, \theta) n(D) dD, \tag{1}$$

where $n(D)\mathrm{d}D$ is the number of particles with a diameter in the range $(D, D + dD)$ per unit volume, A is the effective cross section of incident beam, L is the optical path of the laser beam from the source to the monitoring point, and α is a size parameter defined as $\alpha = \pi D/\lambda$, where λ is the wavelength of the incident beam.

If one assumes a spatial uniform distribution of scattering centres (macromolecules, powder particles, liquid droplets) Equation (1) has the following form:

$$\begin{aligned} I(\theta) &= \frac{cAL}{V} \int_0^\infty i(\alpha, \theta) p(D) dD \\ &= K \int_0^\infty i(\alpha, \theta) p(D) dD \end{aligned} \tag{2}$$

where, $p(D)$ is particle size distribution and $K = \frac{cAL}{V}$, where V is the unit volume.

Furthermore, the expression $P(\alpha, \theta)$ is given by:

$$P(\alpha, \theta) = \left[\frac{3}{U^3}(\sin U - U \cos U)\right]^2 \tag{3}$$

where U is the shape correction factor for a wide range of scattering angles applied to the single particle scattering calculations [11, 18–24] and it is defined as:

$$U = 2\alpha \sin(\theta/2) = \frac{2\pi D}{\lambda} \sin(\theta/2) \tag{3a}$$

Now, we calculate the scattering angles in the range of $(0 - 5$ rad). Note these calculations are just first approximations and they are meant to show only the qualitative behaviour. Quantitative agreement with the experimental results may require more complex models.

For $\theta \to 0$, the expression (3) is given by:

$$P(\alpha, \theta) = \frac{\Delta I_\theta}{\Delta I_{\theta=0^o}} \tag{4}$$

Assuming that $P(\alpha, \theta) \sim i(\alpha, D)$, the integral correction factor can be defined as:

$$P_{\text{int}}(\theta) = \frac{cAL}{V} \int_0^\infty P(\alpha, \theta) p(D) dD = K \int_0^\infty P(\alpha, \theta) p(D) dD \tag{5}$$

The results of our numerical calculations are shown in Figures 1(a–f). The angular dependence of the correction factor for the case of a Gaussian distribution is shown in Figure 1(a) and a uniform distribution in Figure 1(b). The mean value of the particle diameter: 1 μm, 7 μm, 15 μm (Figure 1(a)), and ranges: 1 - 10 μm, 1–50 μm, 1–100 μm are varied in our calculations. The parameters used in the calculations are: $c = 5 * 10^{-4}$ g/cm^3, A = 0.5 mm^2, $\lambda = 632.8$ nm, $L = 5$ cm.

On increasing the mean value of the scattering object size (diameter), the correction factor increases, too. As a consequence, the position of the maximum of the distribution determines the diameter of the objects.

The dependence of the correction parameter for various widths of the distribution are shown in the Figures 1(c–f).

The algorithms to calculate scattering on multi-layer cylindrical geometrical objects

The algorithms to calculate the scattering parameters of different geometrical shapes can be used for many applications. From one point of view, they have to be found as solutions of complex equations. The difficulty is finding the boundary conditions and also agreement with the Maxwell equations. The mathematics is complex but clear, which can not be said for the physics. On the other hand, industrial control of processes, such as drawing optical and metal fibres requires control devices. Some "laser solutions" are already on the market, but further scientific approaches and collaboration are necessary. In addition, to two layer structures, three and

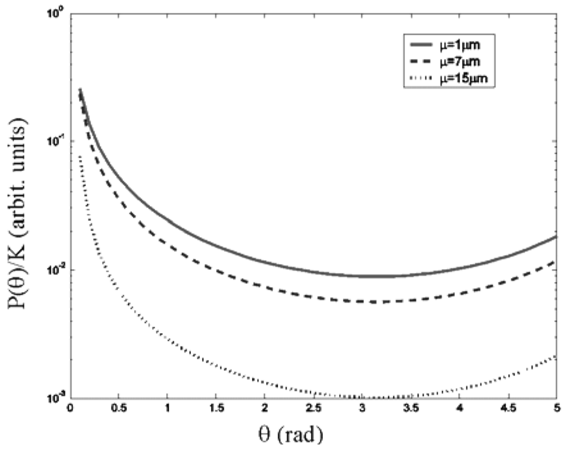

FIGURE 1a
The angular dependence of the correction factor $P_{\text{int}}(\theta)/\text{K}$ in the case of a Gaussian distribution of particle sizes.

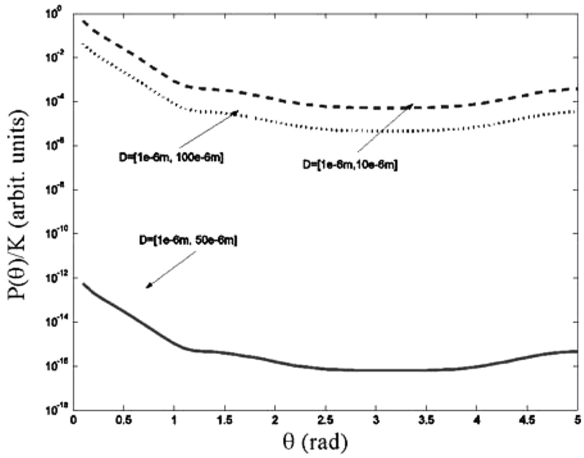

FIGURE 1b
The angular dependence of the correction factor $P_{\text{int}}(\theta)/\text{K}$ in the case of a uniform distribution of particle sizes.

multi-layer structures exist also [33]. Drawing has to be controlled here as well [13, 25–27]. The controlling devices work on the basis of diffraction and scattering figures.

We initiated a study to find a general solution for the scattered intensity for the case of a cylindrical shape. This includes the associated electric field vector, normal to the cylindrical axis. The expression for the scattered

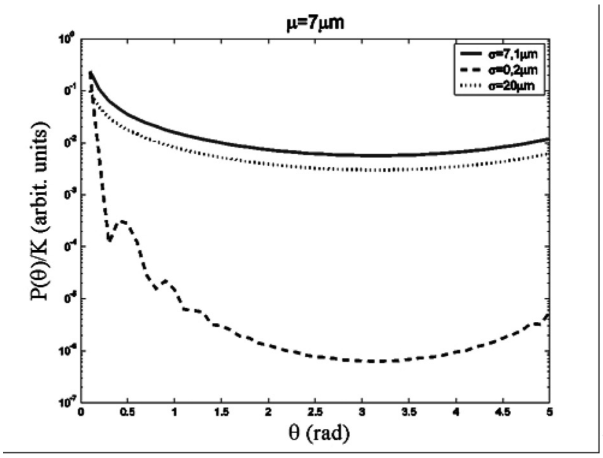

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FIGURE 1c
Influence of σ (dispersion) on the angular dependence of the correction factor $P_{\text{int}}(\theta)$ for $\mu = 7$ μm. Gaussian distribution parameter σ (dispersion) takes the values: 50.0 μm, 7.1 μm and 0.1 μm, respectively.

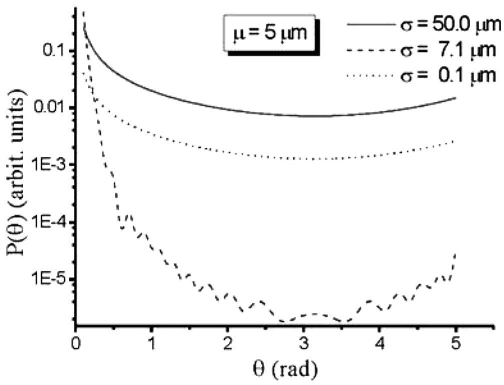


FIGURE 1d
Influence of σ (dispersion) on the angular dependence of the correction factor $P_{\text{int}}(\theta)$ for $\mu = 5$ μm. Gaussian distribution parameter σ (dispersion) takes the values: 50.0 μm, 7.1 μm and 1 μm, respectively.

intensity [25] is:

$$I = \frac{\lambda}{\pi^2 r} \left| b_o + 2 \sum_{m=1}^{\infty} b_m \cos m\psi \right|^2 . \tag{6}$$

The principal difference in expressions for the scattered intensity of a one-layer cylinder and a two-layer cylinder is in the parameters b_m. The

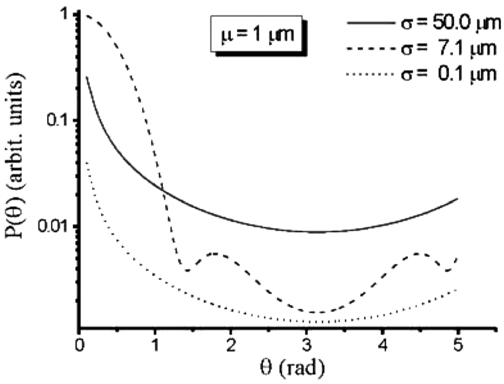


FIGURE 1e
Influence of σ (dispersion) on the angular dependence of the correction factor $P_{int}(\theta)$ for $\mu = 1$ μm. Gaussian distribution parameter σ (dispersion) takes the values: 50.0 μm, 7.1 μm and 0.1 μm, respectively.

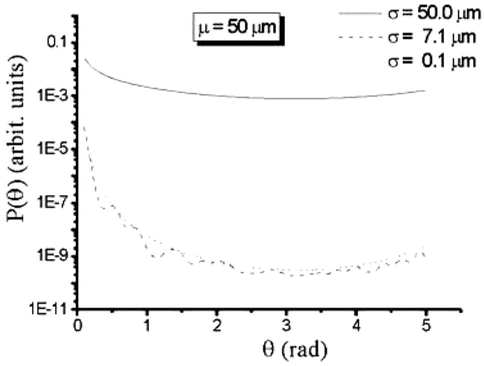


FIGURE 1f
Influence of σ (dispersion) on the angular dependence of the correction factor $P_{int}(\theta)$ for $\mu = 50$ μm. Gaussian distribution parameter σ (dispersion) takes the values: 50.0 μm, 7.1 μm and 0.1 μm, respectively.

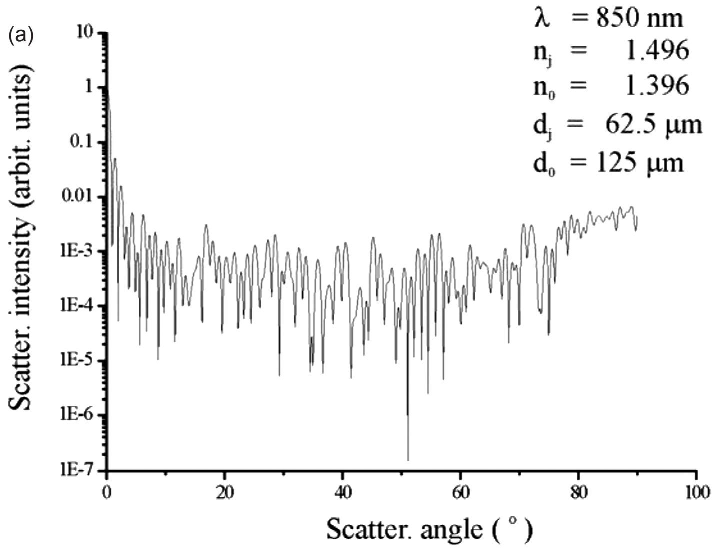
parameters for a one-layer cylinder [11] are:

$$b_m = \frac{\det M_1}{\det M_2} \tag{7}$$

and for a two-layer cylinder:

$$b_m = \frac{J_m(\rho_0)\det M_3 + n_0 J'_m(\rho_0)\det M_4}{H_m(\rho_0)M_3 + n_0 H'_m(\rho_0)M_4} \tag{8}$$

Some details of the equations are given in [19]. The principal calculations depend on the Bessel (Hankel) functions of a definite order [12, 19]. In



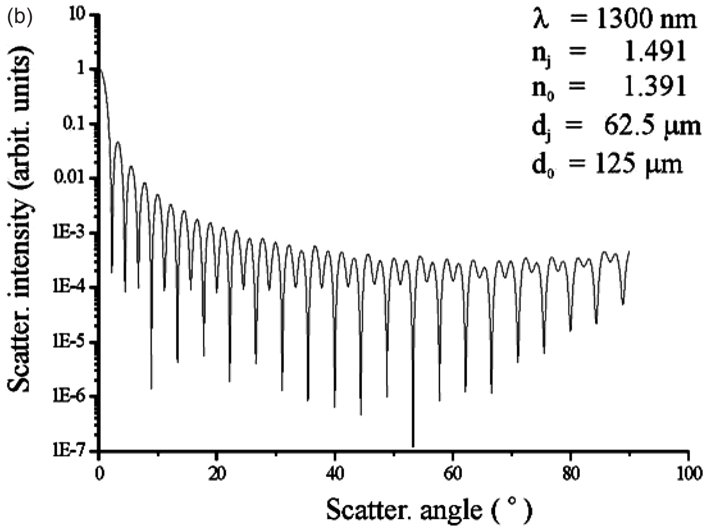


FIGURE 2a
2a and 2b.

Figures 2(a–d) our calculations of the intensities of the scattered light versus scattering angle are shown for 850 nm and 1300 nm and various sizes of two-layer cylinders surrounded by air, i.e., a) $\lambda = 850$ nm, $n_j = 1.496$, $n_0 = 1.396$, $d_j = 62.5$ μm, $d_0 = 125$ μm, b) $\lambda = 1300$ nm, $n_j = 1.491$, $n_0 = 1.391$, $d_j = 62.5$ μm and $d_0 = 125$ μm, c) $\lambda = 850$ nm, $n_j = 1.491$,

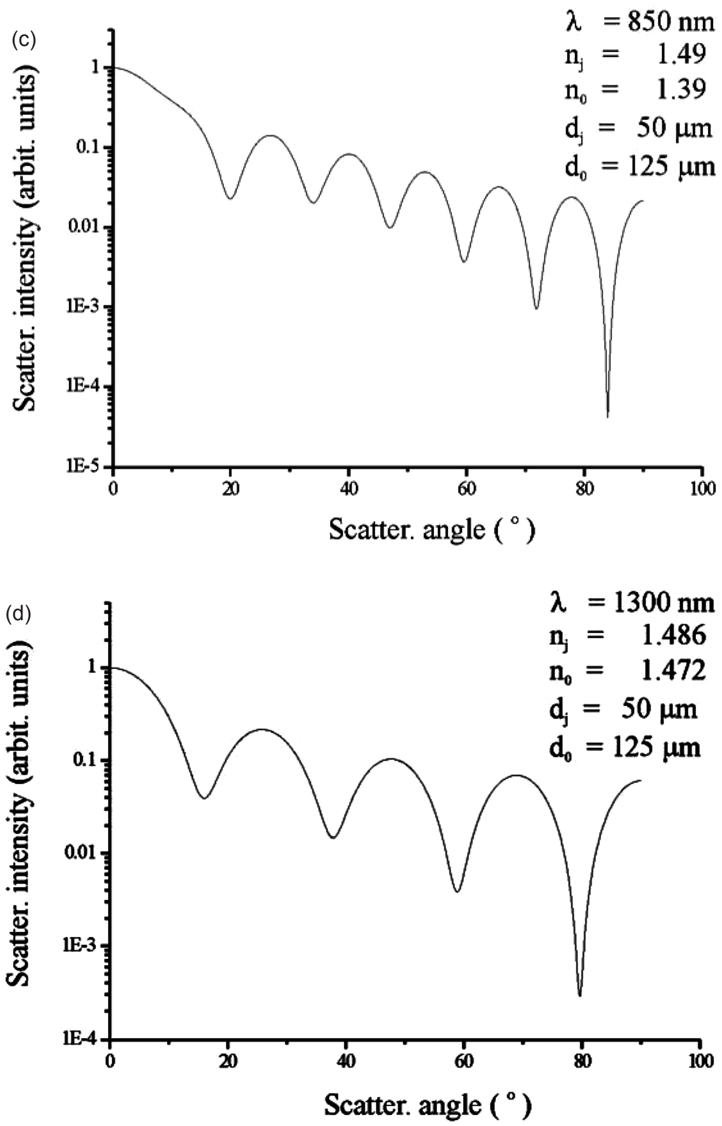


FIGURE 2b
2c and 2d.

$n_0 = 1.391$, $d_j = 50$ μm and $d_0 = 125$ μm, d) $\lambda = 1300$ nm, $n_j = 1.486$, $n_0 = 1.472$, $d_j = 50$ μm and $d_0 = 125$ μm. The designations are after the representation of the geometrical sizes (diameters and respective indices of refraction of "core" and "cladding"). It should be noted that the values selected are those chosen from commercial optical fibres applied in modern telecommunications.

Summation of series

The correct summation presents a second class of problem when considering light scattering. In the light scattering theory there is much mathematical summation of various series. The question whether a series will converge is always important, but as well, it must be understood why and what are the criteria. Hence, we analysed and proved summation of those cases, which are not found in the light scattering literature. Usually, the derivation of the scattering intensity is based on a summation series. We consider that this summation of implemented series has to be discussed.

The intensity of electromagnetic beams scattered by cylindrical objects can be presented by a series which is not convergent, according to the Cauchy definition. The first rigorous definition of the convergence of a series is given by Cauchy, as is accepted today. He had defined a convergence of a series as a convergence of its partial sums. It was found that the class of series, which are convergent in the sense of Cauchy's definition, is too narrow and that it is necessary to change (to extend) the meaning of the convergence. Thus, some series, divergent in an ordinary (Cauchy) sense, can be convergent in a more general sense (the generalized convergence). A real number can be associated using a well-defined procedure to some series divergent in an ordinary sense. This number represents now the sum of such series. After a detailed analysis, we can propose some efficient procedures to prove the summation of a divergent series in an ordinary (classical sense). Thus, we associate one real number to this series. Then, we proved that the series can be summed, according to the approach by G. Frobenius, O. Holder, E. Cesaro and O. Toeplitz [19].

3 PHASE DOPPLER ANEMOMETRY IN PARTICLE SIZING

The configuration Laser Doppler anemometry (LDA/LDV) systems can be used in various tasks and measuring schemes. In addition to the principal role of LDA – measuring of the speed (of fluid flow, particles etc.), the LDA technique measures density, rheological aspects, shape quality etc. Based on scattering and diffraction processes, special functions and the respective technical support, it is possible to measure the size, too.

The Phase Doppler anemometry, [28, 34b)] is a technique, which uses the angular and spatial placement of the components in the measurement system, with possible modular changes, or size of apertures, is able to measure other objects and in this case, the diameter of spherical particles over the range of sub-micro-metre to mm sizes. The particles measured pass through the intersection of two coherent laser beams and scatter the light

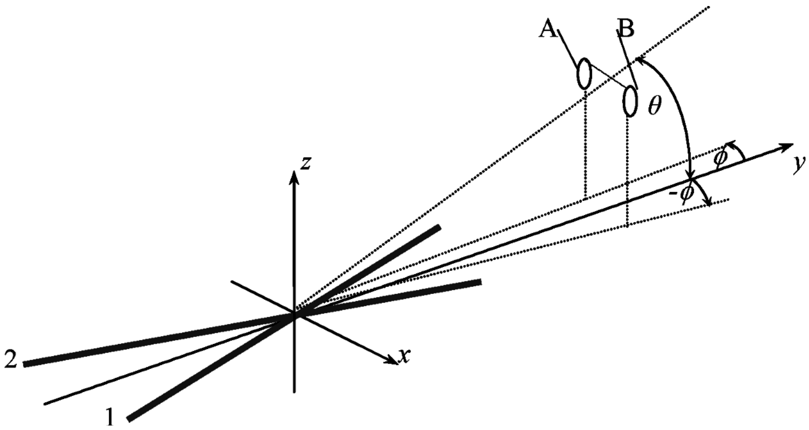


FIGURE 3a
Definition of angles used in the expression of the phase difference between the signals on the photo-detectors A and B.

in all directions and in such a way that the intensity of the scattered light is modulated. Similar to the scattered light intensity, the output signal (on the photo-detector collecting the scattered light) alternates with the frequency of the Doppler shift. The particle velocity can be determined, depending on the Doppler shift frequency. However, the phase of the photo-detector signal at an arbitrary point in space depends on the particle size. It can be shown that the phase difference $\Delta\psi$, between the signals of two photo-detectors situated off-axis in the forward scattering field, is a linear function of the particle radius. In the case of symmetrically placed photo-detectors (A and B in the Figure 3a), the particle radius is given by the expression [17]

$$r = K \cdot \Delta\psi_{AB}, \tag{9}$$

where K is a calibration constant. Its value for the case of transparent spheres can be given as

$$K(\theta, \phi) = \frac{\lambda}{8\pi\left(\sqrt{1+m^2-m\sqrt{2\left(1+\cos\theta\cdot\cos\left(\phi-\frac{\alpha}{2}\right)\right)}}-\sqrt{1+m^2-m\sqrt{2\left(1+\cos\theta\cdot\cos\left(\phi+\frac{\alpha}{2}\right)\right)}}\right)} \tag{10}$$

where m is the refraction index of the particle material relative to the ambient fluid, θ is the scattering angle, and ϕ is the azimuth angle of the photo detector (defined in the Figure 3a).

We carried out a computer simulation of signals produced by light scattered on moving particles and detected by photo-detectors placed at point B (I_B) and at the midpoint between A and B (I_C). The simulation could be the illustration of finding the phase difference of the signals, Figure 3(b).

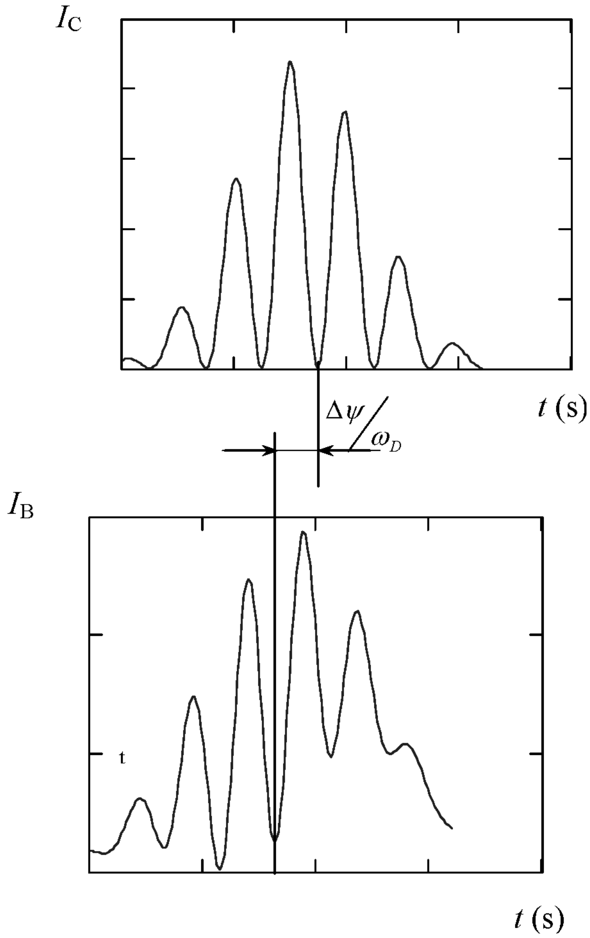


FIGURE 3b
The computer simulated signals of two detectors and their phase difference.

The main source of uncertainty is the non-uniform intensity distribution in the cross-section of the laser beam. It causes the phase difference to be trajectory dependent (trajectory effect) [29]. Considerable distortion of the spherical shape also causes errors in measurement.

4 CONSIDERATION OF MATERIAL DISPERSIONS

The problems considered up to now are those cases without dispersion. In order to illustrate the significance, we shall show modelling of dispersion of dielectric and optical constants and the respective relationships to wavelength.

Taking into account the various relationships between material properties, it is possible to evaluate some of them if others are known. The main group of properties defines the relationship between density and refraction index, density and permitivity, permitivity and refraction index. Some of these relationships are complex, such as the relationship between permitivity (ε) and refraction index (n_D), $x = n_D$

$$\varepsilon = 433.4519 - 563.8899x + 243.0655x^2 - 34.2166x^3 \qquad (11)$$

Some selected analyses on the applicability of experimental data fitting by mathematical functions are demonstrated. The chosen function is

$$f(x) = const + A/x^2 + B/x^4 + \cdots \qquad (12)$$

where $x = \lambda$ and λ is in μm.

The dispersion properties of some materials can be analysed using Hertzberger's approach. For range 0.365–1.014 μm Hertzberger proposes $n = a + b\lambda^2 + CL + dL^2$, where $L = 1/(\lambda^2 - 0.28)$, and λ is in μm. For the IR range Hertzberger proposes another function: $n = A + BL + CL^2 + D\lambda^2 + E\lambda^4$, where $L = 1/(\lambda^2 - 0.28)$, and λ is in μm [30–32].

Some measurements of the dispersion of chosen fibres were performed, Figures 4(a,b).

Measurements were carried out in 'Industry of Cables JAGODINA SCG' in September 2004. The dispersion of Optical Fibres (ALCATEL Type) was measured with a CD3 System Instrument, which is shown in (Figure 4c).

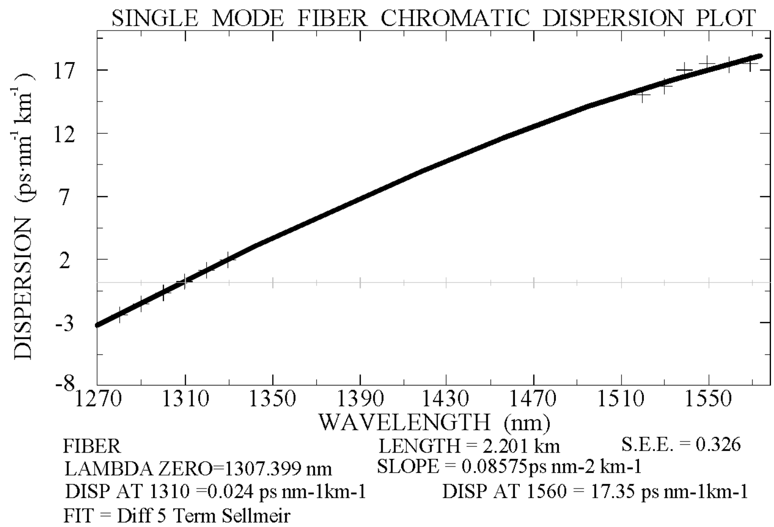


FIGURE 4a

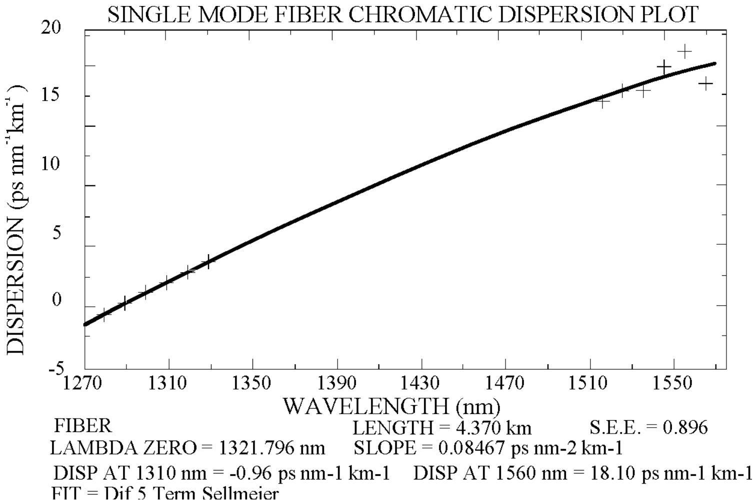


FIGURE 4b

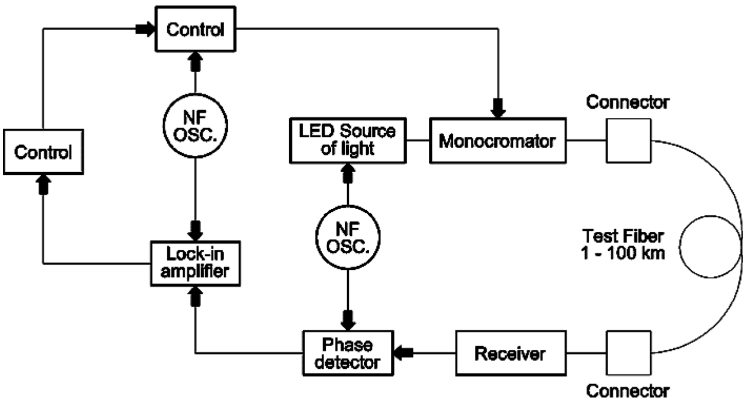


FIGURE 4c
Block-diagram of dispersion measurement system.

It was developed by the 'American Electronic Industries Association Fibre Optic procedure No. 125 (according to IEC 793-1-C5C)'.

The time delay in a mono-mode optical fibre is proportional to the length of the optical fibre and is a function of the wavelength of light. The chromatic dispersion is simply the first derivative of the time delay, depending on the wavelength and is thus:

$$D(\lambda) = \frac{dt}{d\lambda} \cong \frac{\Delta t}{\Delta\lambda} \tag{13}$$

This method is called “the phase drift method”, and the instrument resolution is 1 mm in 100 km of optical cable.

5 CONCLUSION

The conclusion can be two-fold: a general conclusion and a specific conclusion. We start with the specific conclusion. Starting from expression for light scattering intensity on a single particle the cases with particle distributions are derived. The Gaussian and uniform particle size distributions are included, but in the case of independent scatterers any other would be satisfacory. It should be noted, that only large number of scattering centres are included. Consequently, only scattering by the ‘ensemble’ of particles of spherical and cylindrical geometries can be analysed. The results are given as functions of the scattering angle as well as the particle distribution parameter for the particular scattering angle.

In integral scattering, on increasing the mean value of the scattering objects, size and diameter, the correction factor increases, too. It could be concluded that the position of the maximum determines the diameter of the objects. The general conclusion is that $P(\theta)$ for the Gaussian case is approximately that of a parabola. $P(\theta)$ increases with the distribution width. Some kind of anomaly exists for $P(\theta) = 0.7\ \mu$m, independently of the mean parameters. The oscillatory behaviour also exists as a consequence of the numerical procedures applied (depending on the number terms of the series).

The calculation of the scattered light intensity by cylindrical objects, based on non-convergent series in the classic or Cauchy’s sense, as well as other various criteria (of summation) were analysed. These cases include the mathematical task of proving the summations of the series by various convergence criteria. The case of linearly polarised laser irradiation with the polarisation normal to the axis of a homogeneous cylinder has to be considered. Starting from the standard expression for the scattered intensity, a new relationship with introduced special functions has been developed. The principal problem, a mathematical summation of an expression (trigonometric series with Bessel functions as coefficients) and the convergence of the series in classical and general sense are given.

Less standard applications of anemometric measurements in determining the size of scattering objects was analysed. The particle speed and particle size, depend on the Doppler frequency shift and the phase of the photo-detector signals and were analysed and the theoretical expressions derived.

The consideration of dispersion is always a large area of investigation from the point of view of the material alone and especially the significance of fibres in modern telecommunications. As a result of the fibre development, the various types of dispersion could be analysed and discussed. Only some questions of the material dispersion in Cauchy – like equations were analysed in the paper. Generally, the meaning of dispersion includes the relationship between the principal material optical and non-optical constants. The relationship between the dielectric and optical constants and their respective relationships of wavelengths illustrate the significance of dispersion. Dispersion properties of some materials (glass) are analysed by using Hertzberger's approach. Some measurements of the dispersion for chosen fibres were performed. The cases which were analysed before coating fibres are chosen here.

The scattering and diffraction points of view are analysed in this paper. The light intensities provoked by the effects from different obstacles and scattering centres are considered. Various geometries are analysed. Nevertheless, the spherical and cylindrical cases are the object of numerous investigations.

Depending on the theoretical approaches selected angular distributions of integral scattering are obtained. The conclusion that laser scattering (in static and dynamic versions) provides much useful information is still valid. Further sophisticated evaluation with the aid of the developments in mathematical and computer science and supported by new measuring devices often lack assistance in signal processing.

As a conclusion linked to the study of the scattering of cylindrical, multi-layered objects is especially useful in measuring devices to control size, i. e. diameter of fibres in drawing processes. Such devices exist and can measure but the development of the theory is always necessary.

In all cases, special theoretical approaches of various aspects of dispersion linked to optical fibres must also be included. It could be useful in establishing links between the fraction index and their physical and chemical parameters.

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