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## Assessment of the possibility of identifying aqueous suspensions of protein-containing particles by the light scattering matrix

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# Assessment of the possibility of identifying aqueous suspensions of protein-containing particles by the light scattering matrix

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**Abstract.** The possibility of identifying aqueous suspensions of protein-vitamin concentrates (paprin and gaprin) from the measurements of the light scattering matrix has been studied. Based on the real part of the refractive index determined by laser phase microscopy for paprin and gaprin, the scattering matrices of their dispersions in water were modelled. A theoretical analysis of the angular variations of the scattering-matrix elements has shown that the most reliable identification can be practically implemented in the spectral region, where the absorption of light by dispersed particles of at least one of the compared suspensions is small.

## 1 Introduction

Studies of the light scattering matrices of various substances are of interest both from the point of view of fundamental and applied science. The task of recognizing (identifying) disperse media according to their scattering matrices has a great practical significance. The solution of this problem involves both the development of experimental methods for measuring scattering matrices of various media, as well as the development of theoretical models of scattering media and the corresponding numerical methods for solving problems of scattering theory. The availability of experimental data of satisfactory accuracy and an adequate theoretical model that does not require large time resources for the calculation allow one to solve the inverse problem of the scattering theory, that is, the determination of the macro- and microphysical parameters of a dispersed medium. The complexity of the task arises from a large number of factors affecting the elements of the scattering matrix: the size parameter, the type of particle size distribution, the shape and structure of the particles, their orientation, the degree and type of their agglomeration, the complex refractive index ( $n + ik$ ), and the scattering angle ( $\theta$ ).

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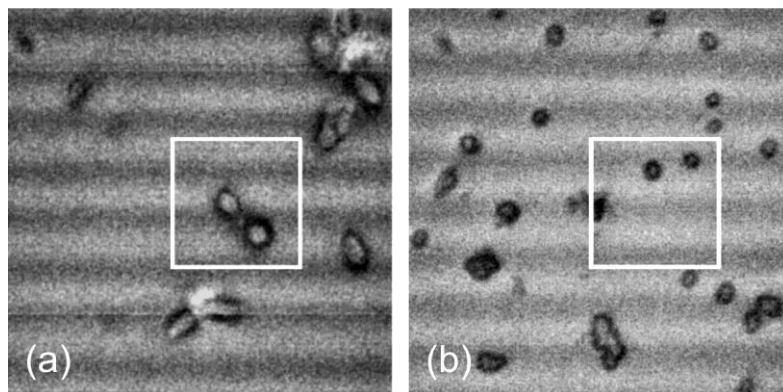


The aim of this study was to determine the conditions when differences in the optical constants of various protein-vitamin concentrates (PVC) can provide the identification of PVCs on the basis of the scattering matrices measured for their aqueous suspensions. For reference, PVC is a dry biomass of feed yeast, grown on oil paraffins (paprin) or natural gas (gaprin) [1]. Paprin contains 40–60 % of protein, and the protein content in gaprin can reach up to 80 %. A specific feature of the problem under consideration is the fact that protein-containing particles suspended in water are characterized by close to unity values of the relative refractive index [2].

The scattering matrix describes the transformation of the polarization state of the incident radiation by the medium. For a macroscopically isotropic medium containing the same number of randomly oriented scatterers and their mirror-symmetric counterparts, the scattering matrix  $\mathbf{F}$  (4x4) has a block-diagonal form [3]. In this case, the elements  $F_{14}$ ,  $F_{41}$ ,  $F_{24}$ ,  $F_{42}$ ,  $F_{31}$ ,  $F_{32}$ ,  $F_{13}$ ,  $F_{23}$  are zero,  $F_{12} = F_{21}$ ,  $F_{34} = -F_{43}$ . The dependence of the element  $F_{11}$  on the scattering angle  $\theta$  describes the scattering indicatrix of unpolarized radiation. For spherical particles,  $F_{22} = F_{11}$  and  $F_{33} = F_{44}$  in the whole range of the scattering angles.

When analyzing the conditions of the identification, it was assumed that the preparation of the suspensions ensures the identity of the average particle sizes of each suspension and allows for a small scatter of the widths of the particle size distribution. In addition, it was believed that the distribution is unimodal and not very wide, and the concentration of suspended particles is such that, on the one hand, a satisfactory signal-to-noise ratio is provided when detecting the radiation scattered by the medium, and, on the other hand, the scattering is single.

Microphotographs of the suspension particles of PVC are shown in Figure 1.



**Fig. 1.** Geometric shape of the particles in the samples of paprin (a) and gaprin (b). The size of the white frame on the images is 8x8 microns.

The micrographic data suggest that the shape of the particles is close to spherical, the ratio of the longitudinal size to the transverse for the particles falls within the range 0.5–2.

Measurements carried out using a phase microscope [4,5] showed that the real part of the refractive index for paprin is 1.46 and that for gaprin is 1.52, which corresponds to the relative refractive index in water  $n_r = 1.1$ –1.14. The imaginary part of the refractive index of proteins, depending on the light wavelength in the visible range, is limited to 0–0.1 [6].

## 2 Simulation results

In the course of the work, the scattering-matrices for suspensions of PVC (paprin and gaprin) were theoretically simulated. It was assumed that the measurement of the matrix elements is possible with a good accuracy in the range of the scattering angles  $10^{\circ}$ – $165^{\circ}$ ,

therefore the differences in the matrix elements are particularly important in this angular range. At scattering angles greater than  $165^{\circ}$ , the measurements cannot be taken because the photoreceiving part of the laser polarimeter setup overlaps the laser radiation. When the scattering angles are less than  $10^{\circ}$ , the portion of the radiation scattered by the windows and facets of the measuring cuvette is large in the recorded scattering intensity. The calculations were performed by the use of a program developed by M.I. Mishchenko according to T-matrix method [3] for an ensemble of randomly oriented spheroids (ellipsoids of revolution). The size distribution of scatterers was considered to be lognormal. The lack of measuring the scattering indicatrix in the whole angular range  $0-180^{\circ}$  does not enable accurate normalization of the  $F_{11}^{(\text{exp})}$  element in accordance with [3]:

$$0.5 \cdot \int_0^{\pi} F_{11}(\theta) \cdot \sin \theta \cdot d\theta = 1 \quad (1)$$

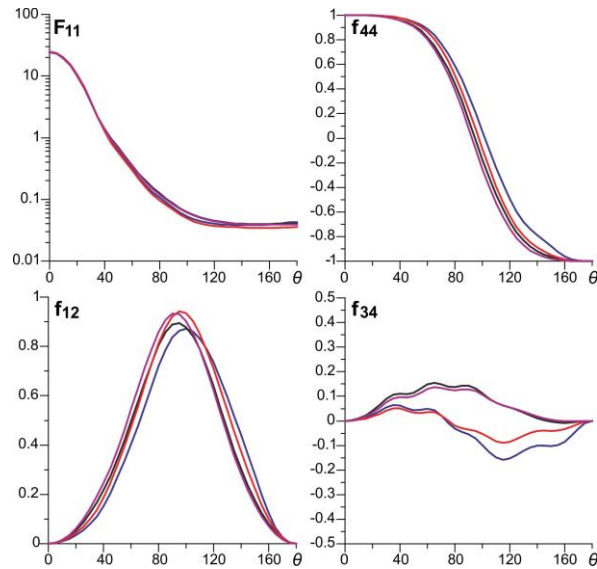
that makes the position of the dependence  $F_{11}^{(\text{exp})}$  undefined along the OY axis. The determining factor affecting the absolute values of  $F_{11}^{(\text{exp})}$  in experimental measurements is the concentration of suspended particles. To compare the experimental dependences of  $F_{11}(\theta)$  among themselves and with the theoretical ones, the experimentally measured values are multiplied by a coefficient  $q$ , which equalizes the values of  $F_{11}$  at an arbitrary scattering angle, usually at  $\theta = 30^{\circ}$  [3]. When analyzing the results obtained, it was assumed that the relative measurement error of the element  $F_{11}$  is 1%, and the absolute measurement error of the rest elements  $f_{ij}$  normalized to  $F_{11}$  ( $f_{ij} = F_{ij}/F_{11}$ ) is 0.03. The scattering matrix of an ensemble of dispersed particles with a random size distribution is determined mainly by the following two parameters of this distribution (the effective size and effective width):

$$r_{\text{eff}} = \frac{\int_0^{\infty} p(r)r^3 dr}{\int_0^{\infty} p(r)r^2 dr}, \quad v_{\text{eff}} = \frac{\int_0^{\infty} p(r)(r - r_{\text{eff}})^2 r^2 dr}{r_{\text{eff}}^2 \int_0^{\infty} p(r)r^2 dr} \quad (2)$$

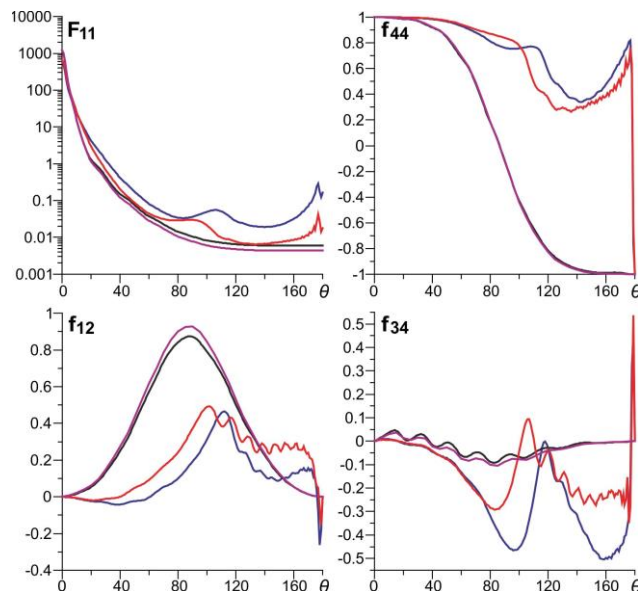
where  $p(r)$  is the probability density distribution. To generalize the simulation results at various wavelengths, the effective size parameter  $X_{\text{eff}} = 2\pi r_{\text{eff}}/\lambda$  is used for the characterization of the size distribution. The simulation was carried out for the particles of fine ( $X_{\text{eff}} = 3$ ) and coarse fraction ( $X_{\text{eff}} = 30$ ). The width of the distribution was varied in the range  $v_{\text{eff}} = 0.1-0.3$ , and the imaginary part of the refractive index ( $k$ ) was in the range  $0-0.1$ . Note that at the relative refractive index of suspended particles close to unity, a change in the width of the distribution leads to small changes in the form of the dependences  $F_{11}(\theta)$ ,  $f_{12}(\theta)$ ,  $f_{44}(\theta)$  and the magnitudes of the matrix elements. An increase in the imaginary part of the refractive index leads to a shift of the dependence of  $f_{44}(\theta)$  and the maximum of  $f_{12}(\theta)$  towards the smaller values of  $\theta$  at the size parameter  $X_{\text{eff}} \leq 30$ .

The results of the scattering-matrix calculations are shown in Figures 2 and 3. From the calculated angular dependences of the matrix elements, it follows that at the wavelengths corresponding to the absence of radiation absorption by PVC particles, the identification of the fine particles is possible via the dependences  $f_{12}(\theta)$  and  $f_{44}(\theta)$ . When measuring the scattering matrix at the wavelengths corresponding to the radiation absorption by both types of PVC, identification, in principle, is possible via the same dependencies, but a slight deterioration in the accuracy of experimental measurements will make it problematic. Changes in the distribution width will not affect this conclusion. At the same time, the noticeable effect of the distribution width on the variation of  $f_{34}(\theta)$  does not allow us to distinguish the type of PVC by this matrix element.

For the particles of the coarse fraction, in the absence of absorption, identification can be realized by the dependences  $F_{11}(\theta)$ ,  $f_{12}(\theta)$ ,  $f_{44}(\theta)$ ,  $f_{34}(\theta)$ . In the case of the absorption of probe radiation by the particles of both suspensions, identification is virtually possible only by the dependences  $F_{11}(\theta)$ . In addition, as follows from Figures 2 and 3, it is more convenient to implement identification on the basis of the scattering matrix in the case when the radiation is not absorbed by the particles of at least one of the compared suspensions.



**Fig. 2.** Dependences of the scattering matrix elements on the scattering angle for the size distribution parameters  $X_{eff} = 3$ ,  $v_{eff} = 0.3$  and the relative complex refractive index:  $n_r = 1.1$ ,  $k = 0$  (red line);  $n_r = 1.14$ ,  $k = 0$  (blue line);  $n_r = 1.1$ ,  $k = 0.1$  (purple line);  $n_r = 1.14$ ,  $k = 0.1$  (black line).



**Fig. 3.** Dependences of the scattering matrix elements on the scattering angle for the size distribution parameters  $X_{eff} = 30$ ,  $v_{eff} = 0.3$  and the relative complex refractive index:  $n_r = 1.1$ ,  $k = 0$  (red line);  $n_r = 1.14$ ,  $k = 0$  (blue line);  $n_r = 1.1$ ,  $k = 0.1$  (purple line);  $n_r = 1.14$ ,  $k = 0.1$  (black line).

The results are in good agreement with the results of studies by other scientists [7-17].

### 3 Conclusions

An example of the protein-vitamin concentrates (paprin and paprin) shows the fundamental possibility of identifying aqueous suspensions of protein-containing substances by measuring their scattering matrices. This kind of identification is implemented more reliably by measurements at the wavelengths corresponding to weak absorption of the probe radiation by the particles of at least one of the suspensions being analyzed. The obtained data can be used in the development of methods for the remote determination of protein-containing substances in dispersed form.

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