SECTION 1. SYNTHESIS, STRUCTURE AND PROPERTIES OF NANOMATERIALS (GRAPHENE, FULLERENES, NANOTUBES, NANOPARTICLES, COMPOSITES ETC.)

OPTICAL CHARACTERIZATION OF 3D DISPERSE SYSTEMS WITH NANO- AND MICRO- PARTICLES: LIGHT SCATTERING MATRIX ELEMENTS

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Abstract – The multiparametric analysis of simultaneous optical data for nano- and micro- particle systems (ensembles, dispersions) by presentation of system characteristics as N-dimensional optical parameter vectors can help to elucidate the nature of particles, the process of particle interactions, the particle share in mixtures of particles and so on. In this paper the application of light scattering matrix elements as vector parameters is shown on the example of influenza virus and colibacillus dispersions. The presentation as N-dimensional optical parameter vectors can serve as innovative research platform for sensing of different particle interfaces including biological ones.

I. INTRODUCTION

Ensembles of nano- and / or micro- particles can be considered as three-dimensional (3*D*) disperse systems (DS) with particles as a disperse phase in dispersive medium [1]. Multiparametric analysis of optical data for 3*D* DS can provide further progress for detailed characterization and control of 3*D* DS with particles of different nature (including biological ones). Taking into account optical theory [1-4] and results of experiments [5-20] can help to elaborate sensing elements for on-line control of 3*D* DS state. Our research [5-19] has investigated different 3*D* DS with nano- and / or micro- particles (with diameter less than 10 micrometers) and has included: a) simultaneous measurements of 3*D* DS by different compatible nondestructive optical methods such as refractometry, absorbance, fluorescence, light scattering (integral and differential, static and dynamic, unpolarized and polarized), and b) solution of inverse optical problem by different methods and technologies of data interpretation by information-statistical theory [21]. The experience suggests that the set of optical parameters of so-called “second class” [11-13, 16-18] is unique for each 3*D* DS [13]. In another words each 3*D* DS can be characterized by *N*-dimensional vector (*ND* vector) in *N*-dimensional space of second class optical parameters [13]. *ND* vectors can reflect in "unobvious" form all peculiarities of 3*D* DS: nature (constituent substances); form, inner and surface structure of particles; distributions of particle size, number, mass, refractive index, etc.; possibilities to aggregation, destruction or interaction with another particles, and so on.

The light scattering matrix elements [2-4] being “second class” parameters by definition (obtained by processing of measured values, dimensionless, mainly independent on the concentration of particles) are very perspective for multiparametric analysis of 3*D* DS. In this paper the application of light scattering matrix elements as *ND* vector parameters (alone and in complex with second class parameters from other optical methods) is shown on the example of such biological 3*D* DS as colibacillus and influenza virus dispersions.

II. MATERIALS AND METHODS

The form of influenza virus particle can be approximated as a homogeneous sphere, but in some cases, the bilayered sphere approximation can be useful. Colibacillus bacterial cells (Escherichia coli, E. coli, colibacillus rods) can be approximated as a homogeneous equivalent volume sphere or as prolate ellipsoids of rotation. In our research the influenza virus strain A1 (H1N1) dispersions with mean diameter of particles ~100 nm and dispersions of colibacillus with equivalent volume sphere mean diameter of cells ~0,6 μm (strain K-802) and ~1,3 μm (strain AB 1157) were used. Due to the great sensitivity of biological objects to the surrounding medium and conditions, it is necessary to use simultaneous measurements for object comparison and to take into account all details of experiments (pH, content of nutrition medium, temperature, etc.).

There is the description of main optical methods used for 3*D* DS characterization (*refractometry*, *fluorescence*, *absorbency*, *integral light scattering*, *differential static* and *dynamic light scattering*) in the previous articles [17, 19]. For the measurements of light scattering matrix elements laser (wavelength 633 nm) self-made installation with detector angles from 60 up to 120 degrees, polarizes and retardation element was used.

III. RESULTS AND DISCUSSION

The Stokes vector **F –** describes the complete polarization properties of a beam of light. The effect of scattering on a beam of light can be represented by the Mueller matrix – *M* (with 16 dimensionless elements – S_{ij}), that transforms the Stokes vector for the incident light – $\mathbf{F}_{inc}$, to the Stokes vector representing the scattered light - $\mathbf{F}_{sc}$ [2,3]:

$$\mathbf{F}_{sc} = M \cdot \mathbf{F}_{inc}, \qquad (1)$$

where: $\mathbf{F}_{inc}$ - the Stokes vector for the incident light, $\mathbf{F}_{sc}$ – the Stokes vector for the scattered light, *M* – 16-element Mueller matrix:

$$M = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{21} & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ S_{41} & S_{42} & S_{43} & S_{44} \end{bmatrix}$$

S_{ij} are functions of the scattering angle and contain all information about the elastic light scattering properties of a particle system at a given wavelength [2-4]. The scattering matrix is determined by the size, shape, symmetry, internal structure and optical properties of the particles in system. In general, all 16 dimensionless elements of the scattering matrix for nonspherical particles can be nonzero and depend on the orientation of the scattering plane. Angular dependence of scattered light depends on the polarization of incident light.

The 3*D* DS state characterization as *ND* vector can be implemented in the *N*-dimensional space of matrix element parameters alone or in the complex with other optical parameters. The first case can be demonstrated on the S_{11} and S_{34} matrix elements data for colibacillus in classical work [20]. The published experimental data about S_{34} / S_{11} angular dependences for two E. coli strains (strain B/r [20, Fig. 5a] and strain K-12 [20, Fig. 5b]) were processing according our *ND*-vector approach: the eight informative parameters was found for dispersion state differentiation in about ten orders and in sign.

In our research, the 3*D* DS state differentiation by *ND* vector of matrix element parameters was used in complex with other optical parameters in order to construct optimal scheme for dispersion on-line control. As example S_{11} data was combined with integral light scattering data for differentiation of two colibacillus strains (K-802 and AB1157) in about one order.

In other example the S_{11} and S_{12} data was combined with integral and static light scattering data for differentiation of influenza virus (strain A1-H1N1) and colibacillus (strain K-802) dispersions. Optical data were presented as the 12*D*, 4*D* and in complex 16*D* vectors. Taking into account the angular dependences of S_{11} (parameters denoted with subscription S) and S_{12} (parameters denoted with subscription P) it is possible to form *ND* vectors $\mathbf{P_S}$ {P_{S1}, $P_{S2}, \ldots$ P_{SN}} and $\mathbf{P_P}$ {P_{P1}, $P_{P2}, \ldots$ P_{PN}} correspondingly (in this example N = 6). The four informative second class optical parameters from integral and differential static light scattering - 4*D* vectors [13], were combined with $\mathbf{P_S}$ and $\mathbf{P_P}$. The complex 16*D* vectors allow differing the state of viral and bacterial dispersions in about seven orders.

IV. CONCLUSION

Optical parameter vector can reflect in "unobvious" form many peculiarities of the system state. 3*D* DS can be characterized and compared one with another by means of *ND* vectors. The vectors can also reflect the changes in the state of mixtures. Due to the fusion of various optical data and by the information statistical theory, it is possible to find the set of informative parameters and to solve the inverse physical problem on the presence of the component of interest in mixtures without any regularization. In this case, the polymodality of particle size distribution is not the obstacle. The number of parameters can be enlarged if to consider angular and wavelength dependences of optical data. *ND* vector approach can be considered as "integral" for the study of whole system as unity with the minimum interference. The presentation of 3*D* DS as *ND* vectors can serve as the innovative research platform for sensing of particle interfaces. It also can demonstrate an awareness of the potential applications for bio- and nano- technology, medicine, industry and for the protection of environment.

REFERENCES

[1] V.J. Klenin, Thermodynamics of Systems Containing Flexible Chain Polymers. Elsevier, 1999.
[2] C.F.Bohren, D.R.Huffman, Absorption and Scattering of Light by Small Particles .Wiley, New York, 1983.
[3] Light Scattering by Nonspherical Particles. Theory, Measurements and Applications, ed. by M.I. Mishchenko, J.W. Hovenier, L.D. Travis, AP, 1999, 690 pp.
[4] F.Ya.Sid'ko, V.N.Lopatin, L.E.Paramonov, Polarization Characteristics of Biological Particles Dispersions. Siberian branch of Nauka publishing house, Novosibirisk, 1990, in Russian.
[5] A. G. Bezrukova //Progr. Colloid Polym. Sci. **93** (1993) 186.
[6] A.G. Bezrukova // Proc. SPIE **3107** (1997) 298.
[7] A. G. Bezrukova //Mater. Res. Soc. Proc. **711** (2002) FF7.9.
[8] O.L. Vlasova and A.G. Bezrukova // Proc. SPIE **5127** (2003) 154.
[9] A.G. Bezrukova // European Cells and Materials Journal **6,** Supplement 1 (2003) 88.
[10] A.G. Bezrukova // Proc. SPIE **5400** (2004) 189.
[11] A.G. Bezrukova // Proc. SPIE **5831** (2005) 112.
[12] A.G. Bezrukova // CD: 2006 Spring National Meeting Conference Proceedings, New York: AIChE, 2006.
[13] A.G. Bezrukova // Proc. SPIE **6253** (2006) 62530C-1
[14] A. Bezrukova, M. Lubomska, P. Magri, M. Rogalski // Proc. SPIE **6597** (2007) 65970M.
[15] A. Bezrukova, M. Lubomska, M. Rogalski // Rev. Adv. Mater. Sci. **20** (2009) 70.
[16] A. G. Bezrukova, Proc. SPIE, **7377** (2009) 73770B-1.
[17] A.G. Bezrukova, O.L. Vlasova // Materials Physics & Mechanics **9** (2010) 167.
[18] A.G. Bezrukova // European Cells and Materials Journal **20,** Supplement 3 (2010) 19.
[19] A.G. Bezrukova, O.L. Vlasova // Materials Physics & Mechanics **13** (2012) 162.
[20] B.V. Bronk, S. D. Druger, J. Czege, W.P. Van De Merwe // Biophysical Journal **69** (1995) 1170.
[21] F.M. Goltsman, Physical Experiment and Statistical Conclusions (Leningrad University Publishing House, Leningrad, 1982), - in Russian.