Acquisition of the pair potential from the structure factor by the model-potential-free method: Study in monodisperse and polydisperse colloidal dispersion systems

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Keywords: Inverse analysis; interaction; density distribution; monodisperse/polydisperse; Boltzmann distribution

Acquisition of the pair potential between the colloidal particles from the measured data of small angle x-ray scattering (SAXS) is an important topic for studies of electric double layers, polymer induced interactions, dispersion stabilities, and aggregations of the colloidal particles. For acquisition of the pair potential, model pair potentials such as Derjaguin-Landau-Verwey-Overbeek (DLVO) potential and Yukawa potential are generally used in the analysis. However, when shape of the real pair potential is not similar to the model pair potential, the model-potential-free analysis should be conducted. In addition, if the real pair potential is obtained from the model-potential-free analysis, it leads to more correct understanding of the interaction. Hence, we recently developed the improved-model-potential-free (IMPF) method for monodisperse colloidal dispersion systems.[1] Calculation of the pair potential without the model potential is difficult, because it is difficult to accurately obtain the structure factor (the input data) up to wide angle. Fortunately, however, the IMPF method has shown the acquisition skill by using the statistical mechanics of liquids (Ornstein-Zernike equation coupled with a closure equation: OZ-closure), Nelder-Mead ranged annealing (NMRA) method, the sparse modeling, and the power law. After development of the IMPF method, we started the challenge of the development of the IMPF method for polydisperse systems also (we call it IMPFP method), because most of the colloidal dispersion systems are polydisperse. Although the program of the IMPFP method is under construction now, we show the simple calculation flow in Fig. 1. In the presentation, we will explain the theories of the IMPF and IMPFP methods in more detail. In addition, the latest calculation results will be also shown.

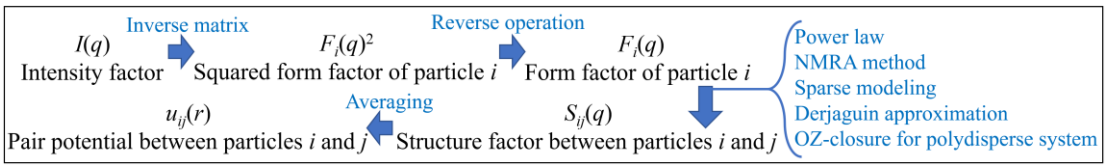

Fig. 1 Calculation flow of the IMPFP method. In the polydisperse colloidal dispersion system, there are many particles with various diameters. The particle diameters are identified with identifier i and j.

1) K. Amano, R. Sawazumi, H. Imamura, T. Sumi, K. Hashimoto, K. Fukami, H. Kitaoka, N. Nishi, and T. Sakka, *Chem. Lett*. **2020**, 49, 1017.