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Hierarchical structure assembled by coordination species in biphasic solvent extraction

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The aim of this study is to elucidate a hierarchical structure of Zr(NO3)4･2TBP in octane, formed in an organic phase of the biphasic solvent extraction system, where TBP is tri-n-butyl phosphate.[1] Toward this end, the methods of extended X-ray adsorption fine structure (EXAFS) and small-angle scattering (SAS), exhibiting a good compatibility in the viewpoint of observing length scale, were employed in this study. EXAFS and SAS are capable of covering the length scales from 0.1–1 nm and 1—100 nm, respectively, reflecting a single coordination structure of Zr(NO3)4･2TBP complex and its self-assembly. Here, note that we need to combine the data obtained for both methods in order to proceed with our understandings of the overall hierarchical structure. First, EXAFS profiles were numerically analyzed in detail in conjunction with a density functional theory calculation, successfully yielding the averaged x-y-z coordinates of Zr(NO3)4･2TBP single complex as a fundamental unit of the self-assembly. We next estimated the contribution of the SAS profile from Zr(NO3)4･2TBP single complex on the basis of the x-y-z coordinates by using Debye function for scattering on an absolute scatter intensity scale. The resultant SAS profiles calculated here exhibited a large difference with the small-angle neutron scattering (SANS) profiles obtained experimentally at q < 1.0 nm-1 (q is the magnitude of the scattering vector), that is, the excess scattering component due to the self-assembling, deviating from that of a single complex, was observed in SANS profiles. In this paper, we would like to report the overall picture of the self-assembled structure into a wide length scale and introduce an original insight into the treatment of EXAFS and SAS profiles.

[1] R. Motokawa et al., J. Phys. Chem. B, vol.116, pp1319-1327, (2012).

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