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The wonderland of absolute scale and contrast variation in small-angle scattering

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A long time ago, Thomas Zemb pointed out that a published study had claimed electron densities corresponding to aluminium in the cores of certain surfactant micelles, something that would have been impossible had absolute-scale modelling been applied together with molecular and concentration constraints. I already appreciated the importance of this approach from my work with contrast-variation SANS at Risø National Laboratory, and I then realized that, to be taken seriously with my SAXS work, I should implement it consistently in my in-house SAXS studies as well. This insight has had a profound impact on my scientific work over the last 25 years.

Thomas Zemb has always demonstrated a deep scientific curiosity, and some of his most characteristic remarks are probably, "This is very interesting (…if it works)," and "They got it totally wrong." Similar sentiments have influenced my own approach to research: "It should be possible to…" , "It could be fun if…", and "This cannot be right".

I will present three projects illustrating this approach to science which I believe align very well with Thomas' perspective . The first concerns analysis of small-angle scattering from precipitates in Al–Li alloys using a polydisperse hard-sphere model(1). This is an early study showing that the use of absolute scale in both SAXS and SANS (combined with a correct interpretation of the theoretical model) enables determination of precipitate stoichiometry. The second study focuses on contrast-variation SANS of AOT micro-emulsions(2), where we demonstrated how contrast variation can disentangle droplet polydispersity and shape fluctuations. This provided an alternative to neutron spin-echo for assessing shape fluctuations and highlighted the importance of controlling isotope effects in contrast-variation experiments, even when the continuous phase is organic. The third study, more technical in nature, shows that for some systems, combining SAXS with static light scattering and absolute-intensity modelling enables efficient (and inexpensive) in-house contrast variation(3,4). A series of PEP–PEO block-copolymer micelles illustrated the complementarity of light and X-ray scattering, providing detailed structural information and insight into the thermodynamics of the systems.

1 Pedersen, J. S. (1993). Small-angle scattering from precipitates: Analysis by use of a polydisperse hard-sphere model. Physical Review B, 47(2), 657.

2 Arleth, L., & Pedersen, J. S. (2001). Droplet polydispersity and shape fluctuations in AOT [bis (2-ethylhexyl) sulfosuccinate sodium salt] microemulsions studied by contrast variation small-angle neutron scattering. Physical Review E, 63(6), 061406.

3 Jensen, G. V., Shi, Q., Hernansanz, M. J., Oliveira, C. L., Deen, G. R., Almdal, K., & Pedersen, J. S. (2011). Structure of PEP–PEO block copolymer micelles: exploiting the complementarity of small-angle X-ray scattering and static light scattering. Applied Crystallography, 44(3), 473-482.

4 Jensen, G. V., Shi, Q., Deen, G. R., Almdal, K., & Pedersen, J. S. (2012). Structures of PEP–PEO Block Copolymer Micelles: Effects of Changing Solvent and PEO Length and Comparison to a Thermodynamic Model. Macromolecules, 45(1), 430-440.

Abstract Title

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