Electronic Supplementary Material (ESI) for Digital Discovery.

Supplementary Information : Metric geometry tools for automatic structure phase map generation

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Examples of Amplitude-Phase distance

In this section, we provide a couple more examples to understand the role of distance in phase mapping intuitively. Figure S1 depicts a similar plot as Figure 1 in the main text but for two SAXS profiles of a BCC that differ in lattice constant by 10%. We observe that, unlike the orange curve in the left panel of Figure 1, the orange curve associated

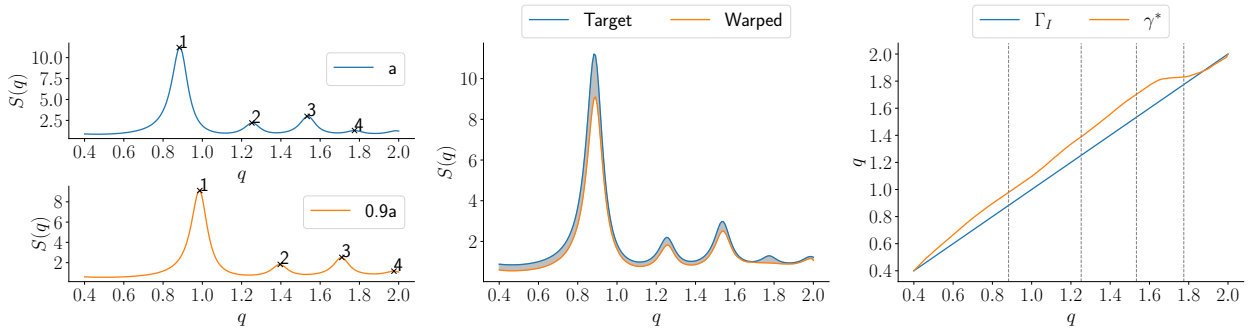

Figure S1: Computation of Amplitude distance between SAXS profile of a BCC phase with a difference in lattice constant that results in shifted peaks. The figure is plotted in the same manner as Figure 1 in the main text.

with warping in Figure S1 assigns a lot less 'distortion' to the aligned curve shown in the middle panel. Finally, we apply a similar analysis to two templates observed in the pluronic case study shown in Figure 3 of the main text. Specially, we try to align the template from panel (D) to that of panel (C) and depict it in a similar manner as Figure S1 in Figure S2. Once again, we observe that by trying to align two very dissimilar profiles, we have added a lot of distortion to the query profile (shown in orange) as shown in the middle panel of Figure S2. Particularly, trying to align a profile with 5 peaks to a profile with a single broad peak resulted in artificial 'bumps' in the query resulting in a distorted shape to the aligned query curve and also the warping function. Moreover, this example also demonstrates that shape is captured beyond peaks that we use for an intuitive explanation. Specifically in Figure S2, note that at lower q-values, the two profiles differ in their shape that was retained and captured after the alignment shown in the middle panel contributing to a shape dissimilarity measure.

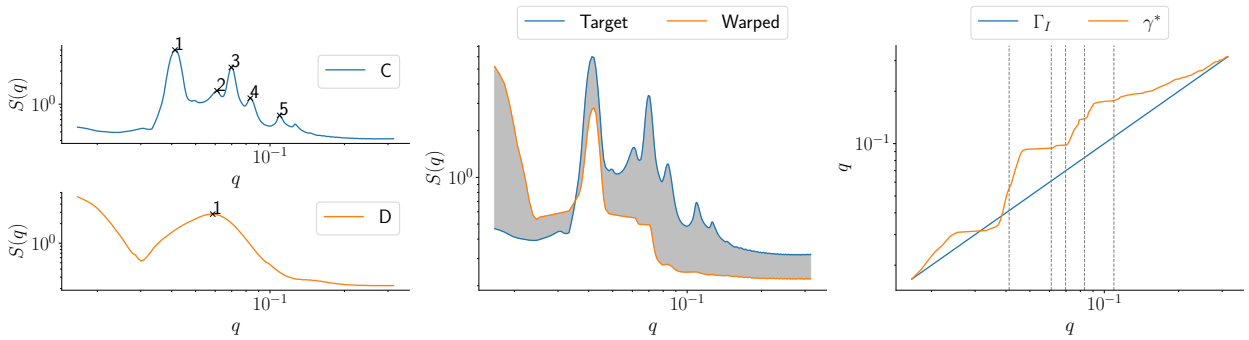

Figure S2: Computation of Amplitude distance between SAXS profiles of templates learned in the pluronic case study shown in Figure 3 of the main text.

Experimental methodology: Sample preparation, processing, and characterization

We synthesized and characterized 505 unique pairs of P123 concentration and temperature in a combinatorial fashion. PEO-PPO-PEO block copolymers were purchased from Sigma Aldrich and PPBT was purchased from Reiki Metals. All polymers were used without further purification or processing. Water was purified with a Millipore Direct Q system immediately before use (electrical resistivity 18.2 M Ω cm). OMIECs were prepared with aqueous PPBT stock solutions and PEO-PPO-PEO in methanol stock solutions. These stock solutions were pipetted using an Opentrons OT-2 liquid handling robot and dried at 60°C overnight. The polymers were vacuumed for 1 hr to remove any remaining solvent. Water was then added to the dried polymers with the OT-2 to reach the desired concentration of PPBT and Pluronic in each sample.

Structural characterization of OMIECs is obtained through high-throughput small-angle scattering (HT-SAXS). HT-SAXS measurements were taken with beamline 12-ID-C at the Advanced Photon Source at Argonne National Laboratory over a Q-range of $0.01 - 1.3\,\text{Å}^{-1}$. Samples were loaded and mounted using a custom-designed aluminum 48-sample well plate sealed between two Kapton windows. HT-SAXS data were collected at room temperature (approximately 26°C) at an exposure time of 1 second. Temperature-controlled HT-SAXS experiments were performed with a few of the OMIEC samples. Capillaries were filled with these samples and loaded onto a capillary stage with a Peltier controller. Samples were measured from 0°C to 100°C. Samples were allowed to sit for 5 minutes in between each measurement to reach the proper temperature.

References