# Understanding diffraction patterns of disordered materials via persistent homology analyses

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The structure of glassy, liquid, and amorphous materials is still not well understood, due to the insufficient structural information from diffraction data. In this talk, attempts are made to understand the origin of diffraction peaks, particularly of the first sharp diffraction peak (FSDP, $Q^1$), the principal peak (PP, $Q^2$), and the third peak ($Q^3$), observed in the measured diffraction patterns of disordered materials whose structure contains tetrahedral motifs. It is confirmed that the FSDP ($Q^1$) is not a signature of the formation of a network, because an FSDP is observed in several tetrahedral molecular liquids. It is found that the PP ($Q^2$) reflects orientational correlations of tetrahedra. $Q^3$, that can be observed in all disordered materials, even in common liquid metals, stems from simple pair correlations. Moreover, information on the topology of disordered materials was revealed by utilizing persistent homology analyses. Figure 1 compares the Si-centric persistent diagram (PD)s for $SiO_2$ glass with three crystalline phases (α-cristobalite, α-quartz and coesite). The PD of silica ($SiO_2$) glass suggests that the shape of rings in the glass is similar to not only to those in the crystalline phase with almost the same density (α-cristobalite), but also to rings present in crystalline phases with higher density (α-quartz and coesite); this is thought to be the signature of disorder. Furthermore, we have succeeded in revealing the differences, in terms of persistent homology, between tetrahedral networks and tetrahedral molecular liquids, and the difference/similarity between liquid and amorphous (glassy) states. Our series of analyses confirmed that a combination of diffraction data and persistent homology analyses is a useful tool for uncovering structural features hidden in halo pattern of disordered materials.

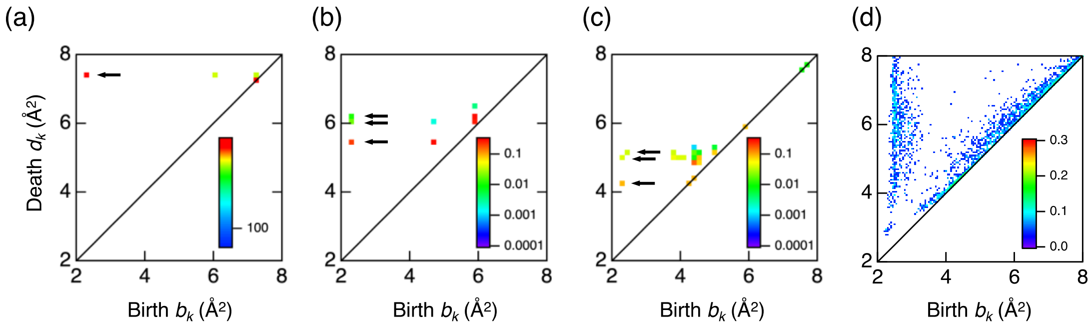


Fig. 1 Si-centric PDs for (a) α-cristobalite, (b) α-quartz, (c) coesite, and (d) $SiO_2$ glass.

## References

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