Scatteirng Pattern Analysis of Polymer Materials using Molecular Dynamics Simulations

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Two-dimensional scattering patterns (2DSPs) provide rich structural information regarding crystallization, domain formation, and void growth (fracture) in polymer materials as well as filler morphologies in polymer nano composites [1]. Molecular dynamics (MD) simulations are promising tools to reveal molecular level behaviors of polymer materials. Recent improvements in computer performance have made it possible to perform MD simulations on systems large enough to calculate 2DSPs that can be compared with the experimerimental results. Recently, we performed large scale simulations for polymer crystallizations and gel network fractures with uniaxial deformations and evaluated their 2DSPs with the circular average.

Figure 1**a,b** shows 2DSPs of crystallized *cis*-1,4-polyisoprene (PI) and *isotactic* polypropyrene (iPP) melts in our MD simulations [2]. To reproduce the cystallizatin of PI and iPP melts (Figure 1**a,b**), we performed united atom MD simulations with TraPPE-UA force field in order to maintain backbone structures that was crucial to the crystallization indudece by stretching. For both PI and iPP, immediately after stretching, only the peak spots due to orientation were observed, although the peaks due to crystallization were not observed. As isothermal crystallization proceeded, the brightness of the peaks due to crystallization increased. We concluded that "orientation" and "crystallization" are separate phenomena.

Figure 1**c** shows 2DSP of stretched polymer network like gels obtained by coarse grained MD simulations using Kremer-Grest model with bond brekage [3]. These bright spots were originated from voids growth under uniaxial stretching. Recently, we confirmed the CGMD simulations with bond brekage is one of the important factors for the generation of hysteresis loop in the SS curve under multicycle deformation. We also investigated the relationship between the progression of network failure and changes in 2DSPs.

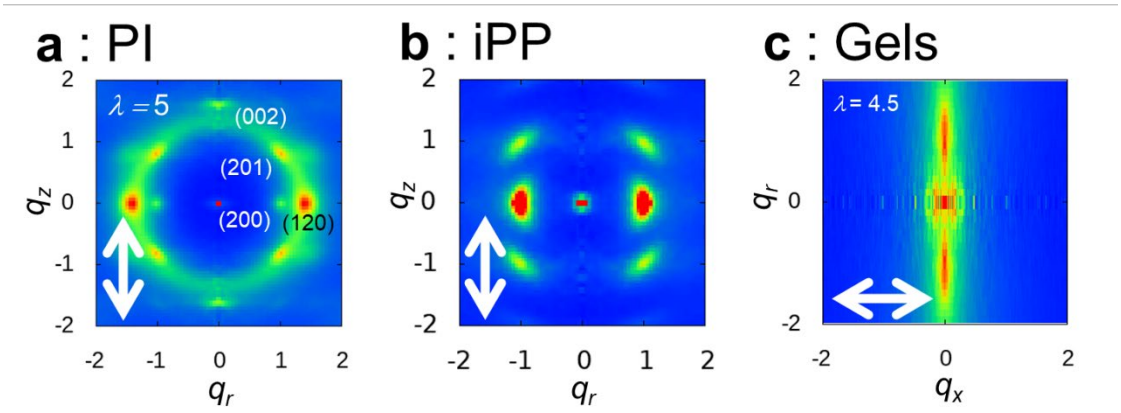

Figure 1: 2DSPs of the crystallized PI (a) and iPP (b), and polymer network (c) under uniaxial deformation.

References

[1] K. Hagita *et al.*, *Macromolecules* **56**, 4457–4467 (2023).
[2] K. Hagita *et al.*, *Under review.*
[3] K. Hagita *et al.*, *Under review.*

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