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Year 2023	**Summary of Thesis**

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(Title)

Refractive index prediction system for transparent polymers

Transparent polymers have been used in various fields of optical technology. When applying polymers as optical materials, the refractive index and dispersion property are important. The refractive index and dispersion are determined by the chemical structure of the repeating unit and the packing state of the molecular chain.

TANIO Laboratory has developed a refractive index prediction system that can calculate the refractive index simply by inputting the type and number of atoms constituting the polymer into a personal computer. **Fig.1** shows the calculation method of the refractive index prediction system. This research aims to improve the adaptability of the prediction system by elucidating and incorporating the unresolved atomic refraction and atomic dispersion into the prediction system. **Table 1** shows the results of the atomic refraction and atomic dispersion of fluorene. The unknown atomic group's refraction and dispersion can be elucidated from the refractive index of a low molecular weight compound with a known molecular

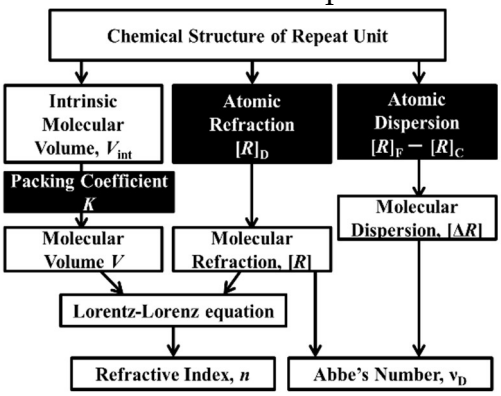


Fig.1 Estimate of refractive index (n) and Abbe's number (ν_D) of optical polymers.

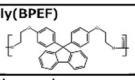
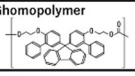
Sample	n_D	n_F	n_C	ρ [g/cm³]	Atomic refraction $[R]_D$	Atomic dispersion $[R]_F - [R]_C$
Poly(BPEF) 	1.6386	1.6578	1.6303	1.25	55.757	2.703
PGhomopolymer 	1.6564	1.6791	1.6477	1.20	62.225	3.656
				Average	58.991	3.180

Table 1 Results of clarification of atomic refraction and atomic dispersion of fluorene.

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weight and density containing that atomic group. By substituting the refractive index, density, and molecular weight of a compound into the Lorentz-Lorenz formula to obtain the molecular refraction and molecular dispersion, and subtracting the sum of the known atomic dispersions from the obtained molecular refractive indices and molecular dispersions, the atomic refractive indices and atomic dispersions of unknown atomic groups can be revealed. The refractive index was measured using a prism coupler (Model 2010, Metricon) for solid samples. And an Abbe refractometer (DR-M2, ATAGO) for liquid samples. Density was determined by the flotation method for solid samples and the density listed on the reagent was used for liquid samples.

These values were incorporated into the prediction system and compared to the literature values for F-PE, a polymer containing fluorene in its structure, to confirm the adaptability of fluorene atomic refraction. As shown in **Fig.2**, the predicted refractive index of F-PE was close (n_D=1.662) to the refractive index described in the literature (n_D=1.66).

By assuming that the atoms composing the polymer are spheres, the intrinsic molecular volume V_{int} of the polymer can be calculated from the atomic volumes of the constituent atoms. However, the actual molecular volume V of a polymer is larger than V_{int} because it contains space due to packing of molecular chains. The molecular volume V is directly related to V_{int} and is expressed as $V = V_{int} / K$. K is called the packing factor, and the closer it is to 1, the denser the packing state of the molecules, and can be calculated from the molecular weight of the repeating unit M_0, the density of the polymer ρ, and the intrinsic molecular volume V_{int}. Within the prediction system, K = 0.68 is used. **Fig.3** shows the results of a close examination of the packing factor K of transparent polymers. A closer look at the packing factor K shows that the plant-derived polymers TO-CNP and starch are greater than 0.68, while PS is smaller than 0.68 at 0.63.

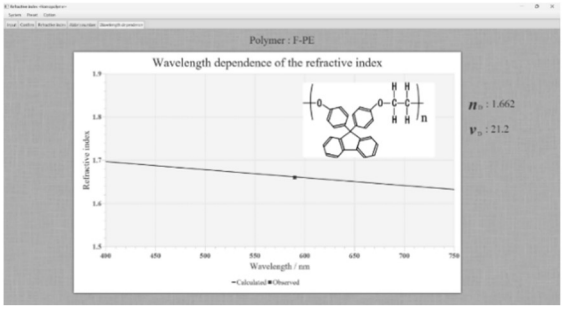

Fig.2 Refractive index prediction for F-PE

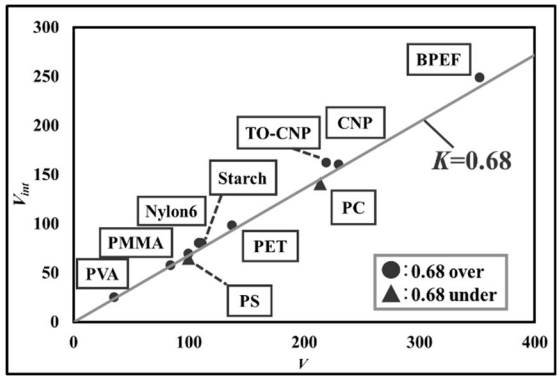

Fig.3 V − V_{int} plot of transparent polymers.

1) Hideyuki HAYASHI, “9,9-Diarylfluorene-Based Poly(alkyl aryl ether)s : Synthesis and Property”, Polymer Journal 41, 609-615 (2009)

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