

Correlation between local dynamics and gas permeability of substituted polyacetylenes by quasielastic neutron scattering

T. Masuda¹, T. Kanaya², R. Inoue² and O. Yamamuro³

¹Department of Polymer Chemistry, Kyoto University, ²Institute for Chemical Research, Kyoto University, ³Institute for Solid State Physics, University of Tokyo

It is well known that some substituted polyacetylenes show high gas permeability among all the examined polymers [1]. We synthesized a variety of substituted polyacetylenes [2,3] and investigated the relationship between gas permeability and side-group structure. Through these studies, we observed that local mobility of side group structure in glassy state plays an important role for gas permeability. In order to confirm this idea, we have investigated local dynamics of several polyacetylene with bulky substitutes using a quasielastic neutron scattering spectrometer AGNES installed at the cold neutron guide C3-2-1.

In this study, we mainly focused on the correlation between local picosecond dynamics and the gas permeability of these polymers. Although glass transition temperatures of investigated polymers are far above room temperature, investigated polymers exhibited quasielastic-like spectrum at room temperature, as shown in Figure 1 (a). It suggests that certain stochastic motion exists even in glassy state. In order to extract the dynamical feature of these polymers, we performed curve fit to the obtained $S(Q, \omega)$. First, we tried to fit with single Lorentzian function, however we failed to describe observed spectrum with single Lorentzian. Hence, we employed two Lorentzian functions and we could describe the observed spectrum well with two Lorentzian functions. We termed broad quasielastic component and narrow quasielastic component as broad component and narrow component, respectively. Neither relaxation rate Γ and fraction A of broad component depend on permeability, however both Γ and A of narrow component exhibited positive correlation with on

permeability coefficient of O_2 . These findings suggest that slow local motion plays major role in gas permeability. This tendency is also visible for the permeability coefficient of O_2 dependence of product of Γ and A for both quasielastic components, as indicated in Figure 1 (b). The behavior of dynamics of these polymers seemed to be explained by the model suggested by Kanaya et al [2]. The detailed analysis is now under progress.

References [1] K. Tsuchihara et al. *Macromolecules*, 25, 8548 (1991). [2] T. Kanaya et al. *Macromolecules*, 35, 5559 (2002).

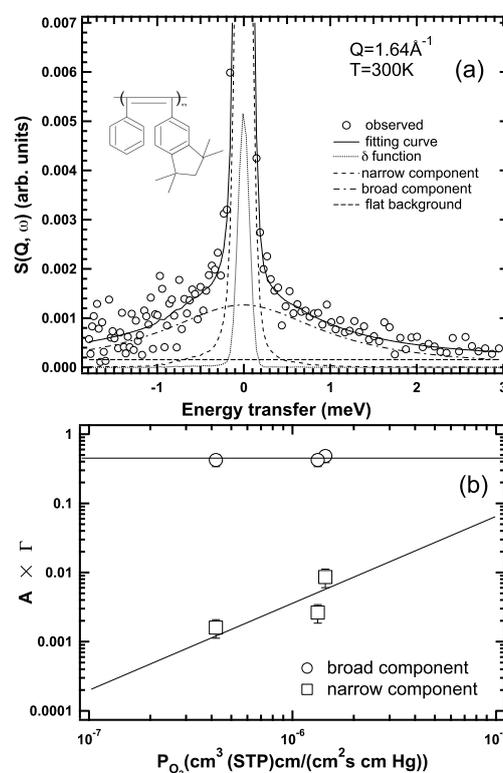


Fig. 1. (a) An example of fits to $S(Q, \omega)$ of one polymer and the quasielastic components were well fitted by two Lorentzians. (b) P_{O_2} dependence of the product of fraction (A) and relaxation rate of both quasielastic components.