

(※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。)

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|  MLF Experimental Report | 提出日 Date of Report 2017/1/27 |
| 課題番号 Project No. 2016B0249 実験課題名 Title of experiment Dynamics of Polyrotaxane in Glassy State 実験責任者名 Name of principal investigator Koichi MAYUMI 所属 Affiliation The University of Tokyo | 装置責任者 Name of responsible person Kenji NAKAJIMA 装置名 Name of Instrument/(BL No.) AMATERAS(BL-14) 実施日 Date of Experiment 2016/11/27-30 |

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)
Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

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| <p>1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.</p> <ul style="list-style-type: none"> - Methoxyethylated polyrotaxane (PR) composed of methoxyethylated cyclodextrin and polyethylene glycol - Methoxyethylated cyclodextrin (CD) |
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| <p>2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。) Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.</p> <p>We investigated the local dynamics of glass-forming polyrotaxane (PR) and cyclodextrin (CD) by means of inelastic neutron scattering. The inelastic neutron scattering experiments were performed using AMATERAS. The incident neutron energies used were 10.5, 5.6, 3.5, 2.4 meV ($\Delta E/E = 3-4\%$). The Q range was from 0.5 \AA^{-1} to 2.5 \AA^{-1}. The temperature at the sample position was varied from 70 K to 380 K.</p> <p>Figure 1 (a) and (b) show the incoherent dynamic structure factors $S(Q,E)$ of CD and PR normalized by the Debye-Waller factor and Bose factor. At around 70 K, both of CD and PR showed boson peaks which are low-frequency vibrational modes characteristic of glassy materials. The boson peak energy and intensity were almost the same for CD and PR, which indicates that the origin of the excitation peak for PR is CDs threaded on polymer chains. At higher temperatures above 100 K, $S(Q,E)$'s of CD and PR deviated from those for 70 K. The amount of the additional scattering increased with temperature. It should be noted that 100 K is much lower than the glass transition temperature (T_g) of CD and PR, 300 K. In the case of polyisobutylene (PIB), $S(Q,E)$ at temperatures below the glass transition temperature of PIB were scaled on a master curve by the normalization with Debye-Waller factor and Bose factor [1]. The considerable amount of the additional scattering for CD and</p> |
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2. 実験方法及び結果(つづき) Experimental method and results (continued)

PR below T_g suggests that CD and PR have a high degree of dynamical freedom even at the low temperatures, which may be correlated with the mechanical toughness of the glassy PR.

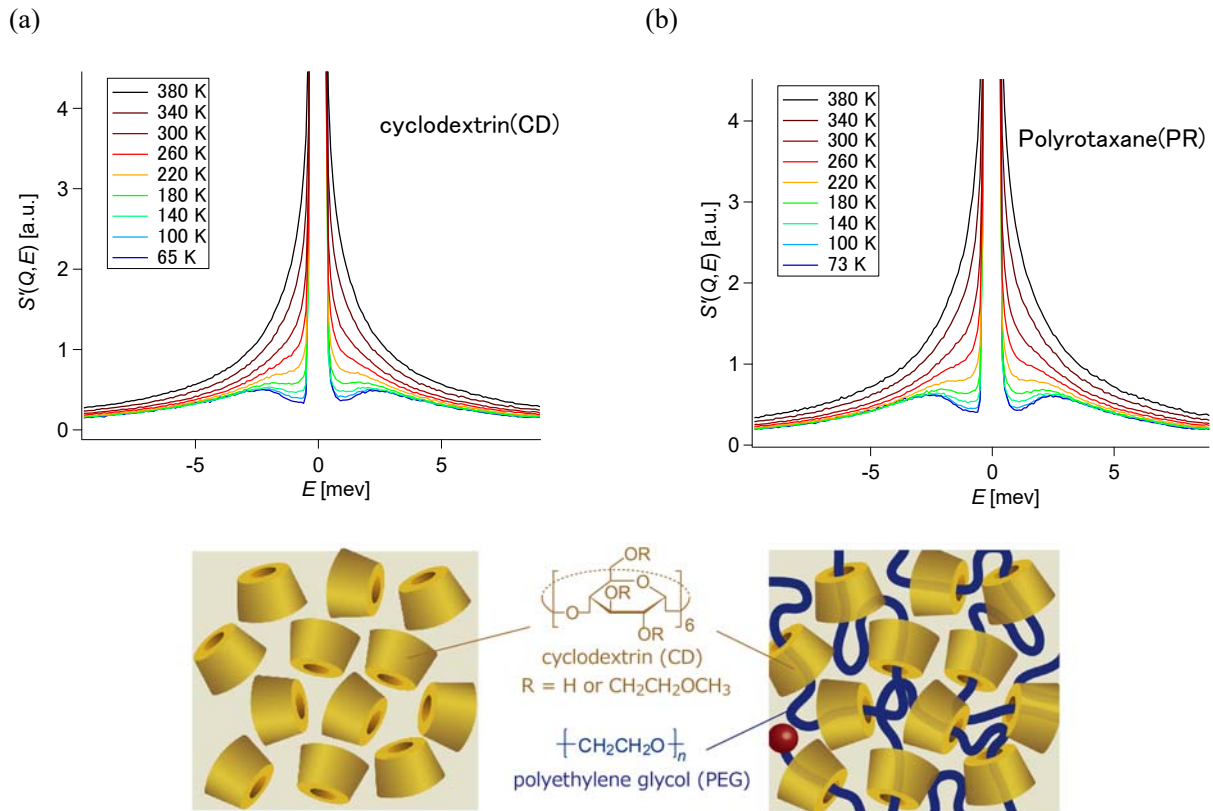


Figure 1. Dynamic structure factors $S(Q,E)$ of (a) CD and (b) PR normalized by the Debye-Waller factor and Bose factor. The data were taken with the incident neutron energy of 10.5 meV.

[1] Frick, B., & Richter, D. (1993). Change of the vibrational dynamics near the glass transition in polyisobutylene: inelastic neutron scattering on a nonfragile polymer. *Physical Review B*, 47(22), 14795.