Study on the Conformability Expression Mechanism of Our Easy Peel-Off Films Using Relaxation Times Measurement and Molecular Dynamics Simulation

Kosuke Iwamoto

Advanced Technology Research & Development Center,
Research & Innovation Promotion Headquarters

1 Abstract

Easy peel-off films can be easily adhered and peeled off at room temperature, leaving no adhesive residue. Due to their convenience, demand for such films is expanding[1)]. An important property of these films is wettability. If wettability is good, they can follow the surface asperity of the adherend with the application of a slight force in a short time and can exhibit sufficient adherence properties. However, in order to control the wettability of the films, it is necessary to predict not only the bulk physical properties but also the behavior of the adhesives at the molecular level, and their design difficulty is high. Therefore, in this study, we developed a new analytical method that can quantify and visualize the relationship between wettability and molecular mobility by using a combination of instrumental analysis and molecular dynamic simulation.

2 Characteristics of the Analysis Technology

- Visualization of nanoscale molecular motions that cannot be observed directly.
- Quantification of the mobility of molecular substructures in materials.
- Prediction of product properties from molecular level behavior.

3 Background of the Development

Easy peel-off films are used in multiple applications, such as preventing damage during processing, storage and transportation of electronic materials, and protecting the surface of smartphones. Hitachi Chemical has developed a pressure-sensitive adhesive for easy peel-off films. Good characteristics are achieved by the use of a monomer with polyethylene oxide (EO) in the side chain. We found that the wettability of the adhesive changes when the EO chain length of the monomer is changed. However, as there is no simple proportional relationship between the EO chain length and wettability, it is difficult to control the properties.

In addition, because there was no correlation between the bulk properties and wettability of adhesives using monomers with different EO chain lengths, it was assumed that the molecular level behavior of the adhesive affects the wettability. However, this assumption was difficult to verify using conventional analytical techniques alone. Therefore, to clarify this mechanism, we tried to develop an analytical method that can visualize the relationship between wettability and molecular mobility.

4 Technical Details

In this study, we developed a new technique that can quantify and visualize the relationship between wettability and molecular mobility by using a combination of instrumental analysis and molecular dynamic simulation. The following shows the results of analyzing the wettability expression mechanism of adhesives for easy peel-off films using the analytical method that we developed.

1) In the molecular dynamic simulation, we created polymer drops of adhesives with different EO chain lengths and visualized their wet spreading behavior onto the adherend. The results are shown in **Figure 1**. It can be seen from **Figure 1** that the model with a short EO chain length has a more rapid initial wet spreading rate than the other models, and has better wettability. **Figure 2** shows the verification results of easy peel-off films that we actually created. When the wettability was

evaluated from the time required for the area where the film and the adherend are in close contact to spread across the adherend, it confirmed the same trend as the simulation results. Furthermore, it was found that extreme wettability values exist with respect to EO chain length.

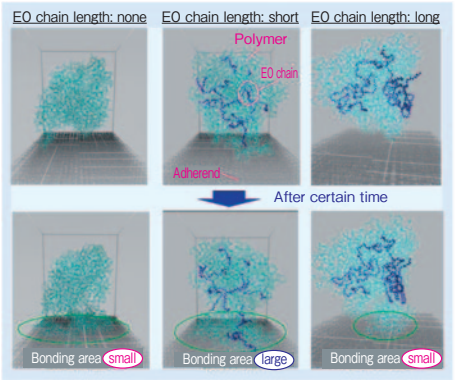
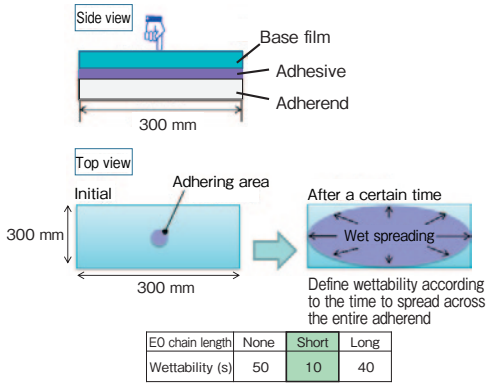


Figure 1 Analysis Result of Wetting Behavior of Adhesives to Adherent by Molecular Dynamics Simulation



EO chain length	None	Short	Long
Wettability (s)	50	10	40

Figure 2 Performance Assessment Method and Results of Wetting Behavior of Each Adhesive

2) The nuclear magnetic resonance apparatus (NMR) can calculate the lattice-spin relaxation time for each molecular substructure. This relaxation time correlates with the mobility of the molecule. It can be said that the longer the relaxation time of the studied adhesive, the higher its molecular mobility is[2]. **Figure 3** shows the change in relaxation time of each part of the EO chain when the temperature changes. From **Figure 3** it can be seen that the amount of change in relaxation time due to temperature rise varies according to the EO chain length. Suggests that the restraint state of the EO chain differs in the adhesives. This is consistent with the results of the molecular dynamic simulation. Focusing on the behavior of the EO chain in **Figure 1**, the short EO chains exist to extend into the polymer and show a behavior that promotes wet spreading of the adhesive. However, the long EO chains aggregate and exhibit behavior that inhibits wet spreading.

3) Based on molecular dynamic simulations and relaxation time measurements, the wettability expression mechanism of the studied samples is summarized in **Figure 4**.

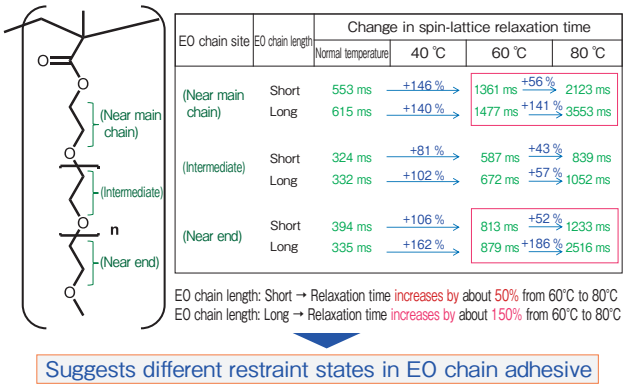


Figure 3 Measurement Results of Spin-lattice Relaxation Times of Polyethylene Oxide Chain Partial Substructures under Heating Conditions

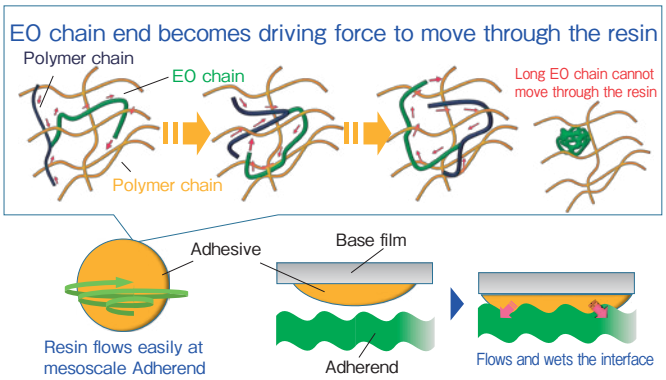


Figure 4 Mechanism of Wettability Triggered by Specific Chain Length of Polyethylene Oxide

5 Future Business Development

- Development of the technology using this method to various adhesives
- Establishment of the expression mechanism for other properties, such as peelability

【References】

1) Current Status and Future Prospects of Functional Polymer Films, Fuji Keizai (2015)

2) T.D.W Claridge: High-Resolution NMR Techniques in Organic Chemistry, Tokyo, Kodansha, Ltd., pp.13-44 (2004)