

Dissolution Mechanism of High Refractive Index Organic Monomer

Daichi Tanaka, Ryutaro Sugawara, Takuro Asaba, Naohiko Ikuma, Dai Shiota

da-tanaka@tok.co.jp

Tokyo Ohka Kogyo Co., Ltd., 1590 Tabata, Samukawa-machi, Koza-gun, Kanagawa, 253-0114, Japan

Keywords: High refractive index material ; Triazine ; Solubility ; Molecular dynamics

ABSTRACT

Recently, triazine monomer has been focused on as a high refractive material. However, this material is often challenged by its insolubility. We clarified the dissolution mechanism by molecular dynamics calculations and designed molecules to improve the solubility.

1 Introduction

High refractive index (HRI) materials are necessary to achieve high functionality in displays. Generally, the refractive index is increased by using inorganic nanoparticles. However, if the film is formed using only the inorganic nanoparticles, voids are formed between the particles, so that the ideal high refractive index cannot be achieved. Therefore, an ideal refractive index is realized by adding organic molecules to fill the space between the particles. Triazine monomer is an organic material with a high refractive index, which is relatively easy to synthesize [1]. However, triazine monomer is often challenged by its insolubility. If the solubility of triazine monomer is improved, it can be widely used as a display material. TOK used molecular dynamics simulation to clarify this insolubility mechanism and synthesized a monomer with improved solubility. Here, we report on the analyzed solubility mechanism.

2 Experiment

Solute is some types of triazine. Solvent is PGMEA and TEGdME. Figure 1 represents one of triazine molecules and solvents.

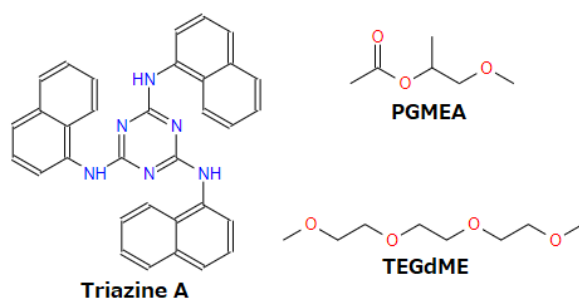


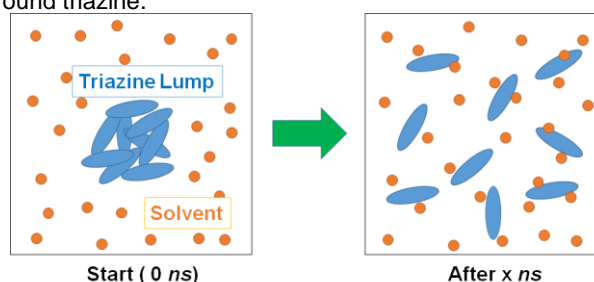
Figure 1 One of triazine molecules and solvents.

2.1 MD Calculation

Fully atomistic MD simulation were performed using LAMMPS (lammmps-12Dec18) [2] and the optimized potentials for liquid simulations (OPLS-AA) [3].

We create triazine lump in vacuum and added to solvent with NPT condition of 373 K, 1 atm and 1 fs timestep (Scheme 1). After some triazine dissolved state obtained, we analyzed its coordination state of solvent molecules to triazine.

Then, we created intentional distributed state and analyzed the coordination state of the solvent molecules around triazine.



Scheme 1

3 Results and Discussion

We obtained triazine dissolution mechanism and were able to dissolve the triazine in the poor solvent.

3.1 MD Calculation

Figure 2 represents the dispersed structure of triazine after the lump was dissolved in solvent. In good solvents, we can see the lumps are decomposing.

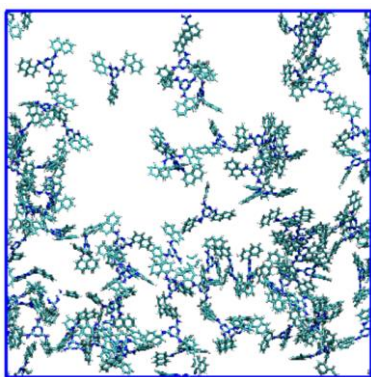


Figure 2 Obtained snapshot which triazine A dissolved. Solvents are hidden for clarity.

Figure 3 represents one of the solvated triazine structure in dissolution after the lump dissolved. We can see that the dissolved triazine has solvent molecules coordinated to the amine part by hydrogen bonds.

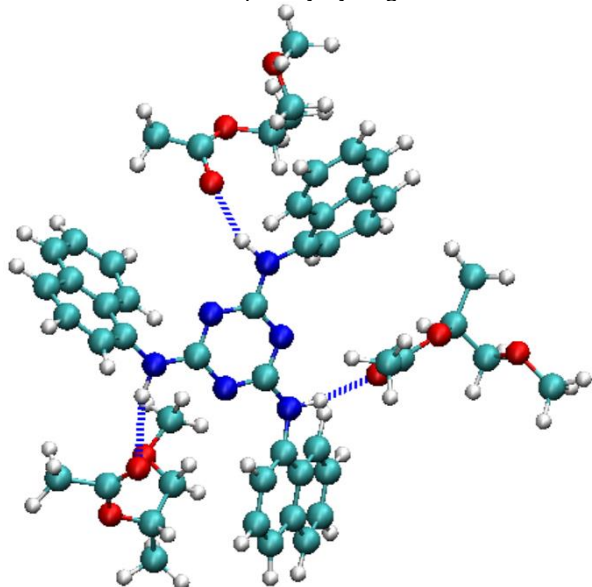


Figure 3 Obtained snapshot which Solvent molecules are coordinated to triazine A.

As expected, the triazine lump did not dissolve in poor solvent. However, intentionally dispersed triazines kept dissolved with the hydrogen bond coordination to the poor solvent. In this case, solvents coordinated structure is same as Figure 3. We will represent a key-parameter for decomposition rather than stability by solvation on the presentation.

Figure 4 represents the dispersion process of lump. We can see that good solvent molecules penetrate through the gap of the triazine lump and finally decompose the lump. Therefore, we can understand that the solubility of triazine can be improved by lowering the planarity and reducing the intermolecular forces to promote the penetration of solvents.

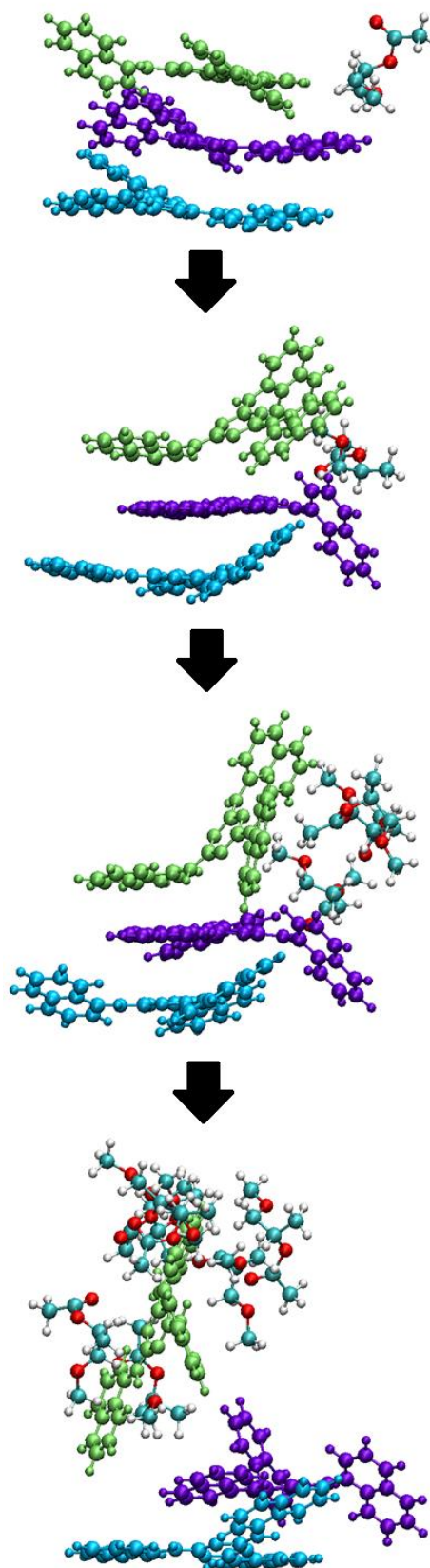


Figure 4 Dispersion process of triazine lump.

3.2 Discussion

Dissolution rate and dissolution stability contribute to the dissolution mechanism. The dissolution rate can be controlled by the three-dimensional structure and the strength of the intermolecular force. The dissolution stability can be controlled by the solvation stability due to the functional group such as hydrogen bonding property. Therefore, it is considered possible to generate a pure dispersion liquid, regardless of the dissolution rate, by performing solvent substitution and so on.

4 Conclusions

We found that the structure of the triazine coordinated to the solvent is the same regardless of the solubility. However, the difference in solubility is caused by the different cohesive between the triazine monomers. Therefore, we confirmed that the solubility could be improved by changing the functional groups to reduce the planarity and intermolecular cohesive forces.

References

- [1] H. J. Lee, B. D. Sarwade, J. Park, E. Kim, "Synthesis of new photopolymeric methacrylate thioether with s-triazine ring for holographic recording", *Optical Materials*, 30, pp. 637-644 (2007).
- [2] <https://www.lammps.org/>
- [3] Jorgensen WL, Tirado-Rives J: "The OPLS Force Field for Proteins. Energy Minimizations for Crystals of Cyclic Peptides and Crambin." *J. Am. Chem. Soc.* 110, :pp. 1657–1666 (1988).