

# The molecular mechanism of the thermo-responsive shape memory effect of self-assembled poly-{2,5-bis[(4-butoxyphenyl)oxycarbonyl]styrene} fiber

Li-Ying Wan<sup>1</sup> · Rong-Mei Han<sup>1</sup> · Zi-Han Wan<sup>1</sup>

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**Abstract** A new molecular mechanism is proposed to explain the shape memory effect of mesogen-jacketed liquid crystalline polymer fiber—poly-{2,5-bis[(4-butoxyphenyl)oxycarbonyl]styrene} (PBPCS) fiber—designed in the molecular level. Due to the strong “coupling effect” between flexible backbone and rigid side mesogens, the molecular structure of PBPCS can be regarded as “dual chains” model that is constituted by a flexible backbone chain and a rigid side chain in parallel. The flexible backbone chains are reversible above the transition temperature and act as a switch structure, the physically cross-linked points caused by the  $\pi$ - $\pi$  weak interactions between rigid side mesogens are responsible for memorizing a shape function and act as a fixing structure; therefore, the switch structure (flexible backbone) and the fixing structure (rigid mesogens) are found in each macromolecular chain. Furthermore, the shape memory behavior of PBPCS fibers is discussed by a viscoelastic molecular model consisting of two Maxwell models in parallel, the obtained theoretical values by “dual chains” model was in agreement with experimental results, very well. The viscoelastic molecular model described for shape memory process was correlated to the molecular mechanism explained for shape memory effect. This work provides a new idea and significant approach for design of new shape memory polymers.

**Keywords** Shape memory effect · Switch structure · Fixing structure · Coupling effect · “Dual chains” model

✉ Li-Ying Wan  
wlygood@nchu.edu.cn

<sup>1</sup> School of Material Science and Engineering, Nanchang Hangkong University, Nanchang 330069, Jiangxi, China

## Introduction

Traditionally, shape memory materials (SMMs) include shape memory alloys (SMAs), shape memory polymers (SMPs) and some specially designed shape memory hybrids (SMHs) [1]. After being deformed, SMMs can recover their original shapes when the right stimulus is applied, which is known as the shape memory effect (SME) [2]. The SMPs have attracted much interest because of their light weight, high shape recovery, low cost and ease of fabrication and processing as compared with SMAs. In recent years, SMPs and their composites have been used in a wide range of new applications such as functional nanocomposites, controlled drug delivery, targeted gene delivery and new biomimetic self-healing systems [3, 4].

In SMPs, the shape memory process is simply presented as follows: the original shape is deformed by external factors (for example heating [5, 6], cooling [7], light [8, 9], magnetism [10, 11] and electricity [12]), the shape is fixed as temporary deformation and then SMP is returned to its permanent shape again. A SMP usually has two components consists of fixing and reversible parts that the shape is maintained by fixing component and changed by reversible component [13]; therefore, the dual-domain system is the mechanism for the SME in SMPs. Nevertheless, shape memory effects of different types of SMPs (such as chemical and physical cross-linked, self-assembly, nanocomposites, etc.) are different because of various underlying mechanisms [14–16]. In order to give a correct and comprehensive simulation of shape memory, we must make an in-depth study on the specific molecular mechanism during the SMP deformation process.

In general, the exact working mechanisms behind various shape memory features in response to different stimuli [17, 18]. Three working mechanisms including dual state