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# Liquid-crystalline ordering in rod–coil diblock copolymers studied by mesoscale simulations

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Using mesoscale dissipative particle dynamics (DPD) simulations, which ignore all atomistic details, we show the formation of lamella mesophases by cooling a fully disordered system composed of symmetric ($A_7B_7$) rod–coil diblock copolymers. Equilibration is achieved very rapidly using DPD, and isotropic, smectic A and crystalline phases of the rod-like blocks can be observed either by heating or cooling. An interesting pseudo-smectic phase can be characterized when the order–disorder transition temperature is above the clearing temperature. This phase gradually fades into a normal microphase-separated structure as the system is heated through the clearing temperature. Simulations of pure rods, however, show the formation of isotropic, nematic, smectic A and crystalline phases.

**Keywords: rod–coil copolymer; liquid crystal; mesoscale simulation; dissipative particle dynamics**

## 1. Introduction

Microphase ordering in block copolymers and mesophase formation in thermotropic liquid crystals are two examples of phenomena that manifest themselves primarily on mesoscopic length- and time-scales. Both processes occur in a large class of liquid-crystal molecules and polymers of practical interest where flexible tails are attached to one or more rigid blocks (Kelker & Hatz 1980). There have been several recent experimental (Chen *et al.* 1996; Jenekhe & Chen 1998, 1999; Lee *et al.* 2001) and theoretical (Duchs & Sullivan 2000; Matsen & Barrett 1998; Reenders & ten Brinke 2002; Semenov 1991; Semenov & Vasilenko 1986) studies aimed at understanding the interplay between microphase ordering and mesophase transitions.

Fifty years ago, Onsager (1949) showed that long rod-like particles, interacting only through excluded-volume interactions, form a nematic phase upon increasing the density. Since then, many computer simulations of liquid-crystal behaviour have been performed using hard-core models, such as spherocylinders and the Gay–Berne

One contribution of 21 to a Theme 'Connecting scales: micro, meso and macro processes'.