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Citation	物性研究 (2006), 87(1): 174-175
Issue Date	2006-10-20
URL	http://hdl.handle.net/2433/110590
Right	
Type	Departmental Bulletin Paper
Textversion	publisher

Single chain distributions at the interface in micro phase separated structures obtained by self consistent field calculations

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昨年度、3次元透過型電子顕微鏡により得られた3次元ラメラ構造上で自己無撞着場計算を行い、実験で得られた構造に対してさらに詳細な鎖の情報が得られる事を示した。本発表では、ブロックポリマーによって得られる幾つかのミクロ相分離構造に対して上の方法を適用し、鎖の伸び等に関して解析を行ったので報告する。

1 Introduction

In the previous workshop, we show the results of the single chain distribbutions in the real three dimensional (3D) phase separated structures by combining 3D transmissin electon microscopy (TEM) and 3D self consistent field (SCF) simulations. We applied this method to the problem of the several kinds of phase separated structures obtained by 3DTEM. This method has the advantage of being easily able to construct the initial structures for SCF simulations, which exists as a real one.

2 Method

3D TEM image is converted to the initial structures of SCF simulations using the imaging interface to the platform of the OCTA, which we call as "Gourmet." Using this interface, we make the converter program from the sliced image files to the volume fraction data. The original 3D TEM structures are observed by Jinnai et al, and the sample is the micro phase separated structure of polystyrene-polyisoprene (PS-PI) block copolymer.

Using the converted structures, we perform the self consistent field simulation. In this simulation, the mean field potential, which is suitable for the given density profile, is estimated. It is noted that in this simulations the parameters, such as χ, N, and length scales, can be estimated from the condition of experiments. Therefore this simulation is no parameter simulations.

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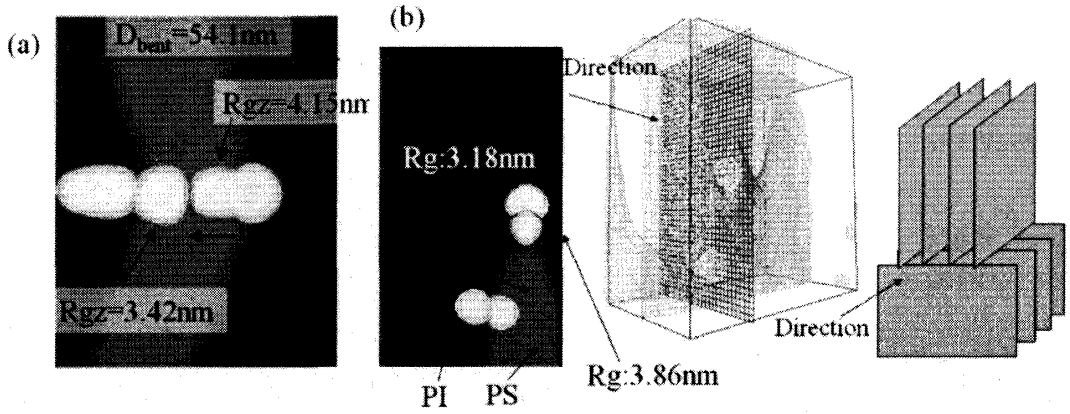

Figure 1: Results of SCF simulations. (a) and (b) show the single chain distributions at the grain boundary, (a) bended lamella and (b) scherk surface, respectively.

3 Results

Figure 1 shows the single chain distribution in the two kinds of grain boundaries, (a) bended lamellar structures and (b) scherk surface, respectively. Fig.1(a) and (b) is obtained by SCF simulation. The junctions shown in Fig. 1 is fixed at the interface of PI and PI domains. From the result of single chain distributions, a chain stretches to the vertical direction to the interface between PS and PI. The length of the stretched chain can be estimated by the gyration radius of each blocks, and these are shown in Fig. 1. Details of the analysis in this study will be shown in the presetation.

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