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Self-organization of BaF_2 Single Crystal Film under a Compressed Langmuir Monolayer

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Self-organization of BaF_2 Single Crystal Film under a Compressed Langmuir Monolayer

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Self-organization of BaF_2 single crystal film under a compressed monolayer of behenic acid (BA) has been investigated by using X-ray diffraction (XRD) and scanning electron microscopy (SEM). The experimental results indicated the (100)-oriented single crystal film of BaF_2 was formed under the BA monolayer. The relation between the BaF_2 single crystal and the monolayer was discussed.

Keywords Self-organization; BaF_2 single crystal film; Langmuir monolayer

INTRODUCTION

Control over crystallization is an important requirement in the preparation of the advanced inorganic materials. Recently, a series of relevant techniques have been developed. One of them is the Langmuir monolayer as potential template for the oriented nucleation of inorganic crystals[1-2]. By this method, it is possible to obtain the desired crystal face and realize the multilayer assembly. Here, we have reported the self-organization of BaF_2 single crystal film under a compressed monolayer of behenic acid.

EXPERIMENTAL SECTION

The BaF_2 supersaturated solution (S=10) was prepared by mixing $Ba(NO_3)_2$ with NH_4F. The filtered solution as subphase was transferred

into a trough of LB system (KSV-5000 Finland). The solution of behenic acid (1mg/mL in chloroform) was spread on the subphase. The monolayer was compressed to the targeted surface pressure (35mN/m). After keeping the surface pressure for 25min. Crystals grown under monolayer were transferred onto the hydrophilic glass substrate in Y type for SEM (JXA-840) and XRD (D/max-IIIA, Rigaku, CuKα).

RESULTS AND DISCUSSION

In the absence of monolayer, the saturated solution of BaF_2 has been placed for 1.5 h. The majority of crystals were located at the bottom of the trough as a result of sedimentation. XRD measurement of crystals indicated several groups of diffraction peaks, and the strongest diffraction peak corresponds to the crystal face (111) (Figure 1a).

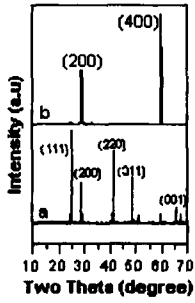

FIGURE 1 XRD images of BaF_2 crystals
(a) crystals at the bottom of trough
(b) crystals grown under monolayer

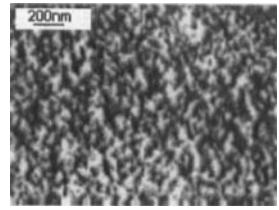

FIGURE 2 SEM micrograph of BaF_2 crystals grown under monolayer

However, in the presence of BA monolayer, nucleation preferentially occurred at the monolayer-subphase interface. XRD analysis of crystal showed only the (200) and (400) reflections, thus indicating that the crystallites are (100)-oriented (Figure 1b). Viewed in larger scope by

using SEM, an even thin film of BaF_2 single crystal was formed (Figure 2). These results reveal that self-organization of BaF_2 single crystal film can be achieved by Langmuir monolayer as inductive template.

Barium fluoride is known to crystallize in a cubic crystalline lattice with a lattice constant of a= 0.62nm. Atomic coordinates are (0 0 0), (0 1/2 1/2), (1/2 0 1/2) and (1/2 1/2 0) for Ba atom and (1/4 1/4 1/4) and (3/4 3/4 3/4) for F atom. Drawing of the (100) projection of Barium atoms is shown in Figure 3a. The calculated distance between the closest Ba-Ba along $(0\bar{1}3)$ direction is 0.98nm. On the other hand, according to the previous reports[3-4] we assume that the BA monolayer also adopts hexagonal lattices under similar conditions (Figure 3b). Using the experimentally determined value for the surface area of one BA molecule ($0.204nm^2$), the lattice constant and the $d_{(100)}$ spacing of the monolayer were calculated to be 0.49nm and 0.42nm, respectively.

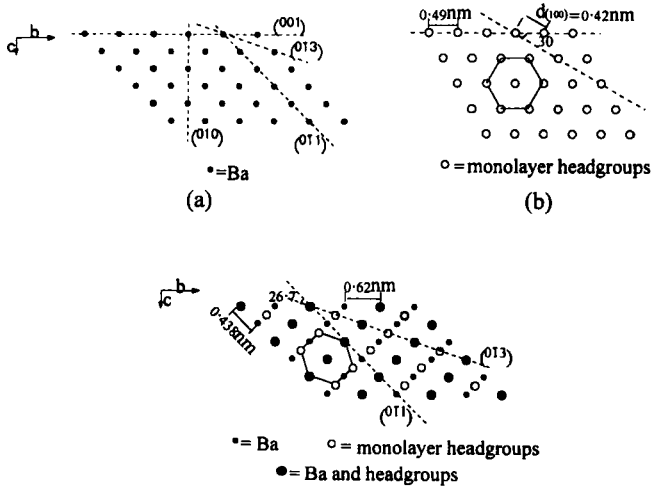

FIGURE 3 (a) Two-dimensional drawing of (100) face of BaF_2 crystal. (b) Two-dimensional packing of BA monolayer headgroups. (c) Schematic two-dimensional representation of the proposed overlap between Ba atoms and BA monolayer headgroups

By simulation techniques, we have found that rhombic distortion of the 30° to 26.6°(the angle between $(0\bar{1}3)$ and $(0\bar{1}1)$) provides a much better matching in two dimension. The Ba-Ba distance (0.98nm) along $(0\bar{1}3)$ direction is 2 times that of the interheadgroup spacing (0.485nm). And the distances between the closest Ba-Ba atoms (0.438nm) along the $(0\bar{1}1)$ direction of the (100) face of BaF_2 crystal fits the $d_{(100)}$ plane to the network spacing of the BA monolayer (0.42nm). A feasible arrangement is shown in Figure 3c. The figure indicated that the BA monolayer assumed pseudo-hexagonal lattice at the air-subphase interface. This also implies the pseudo-hexagonal packing arrangement of the BA monolayer generated a template for the oriented nucleation of BaF_2 crystals on the (100) face and its subsequent growth.

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