Observation on structure in the surface region of cocoa butter, POP, SOS and POS by X-ray diffraction
Yoshihito Uozaki, Yusuke Hayashi, Hikaru Terauchi, Isao Takahashi
Kwansei Gakuin University, Faculty of Science and Technology, Gakuen-2-1, Sanda, Hyogo, 669-1337, Japan, E-mail: cow88323@yahoo.co.jp

Cocoa butter, prepared from ground roasted cacao beans, has six polymorphs characterized by different melting points in thermal analysis. It is known to consist of several oils and fats, e.g., POP (sn-1,3-dipalmitoyl-2-oleoylglycerol), SOS (sn-1,3-dialmitoyl-2-stearoyl-glycerol) and POS (1,3-rac-palmitoyl-stearooyl-2-oleoylglycerol), etc. Since there is some resemblance in molecular structure among them, POP, SOS and POS exhibit six or five polymorphs like cocoa butter. They are also known to acquire stable structures throughout phase transformation via quasi-stable polymorphisms. In the present study, we observe structures in surface region to a depth of 10nm from the surface and those of thin films of polymorphisms of POP, SOS, POS and natural cocoa butter by surface-sensitive X-ray diffraction techniques. The aim of our research is to clarify the peculiar molecular interactions and structures emerging only in the surface and thin films, which would also serve as basic information on melting and oxidation of chocolate. X-ray reflectivity (XR) and grazing incidence X-ray diffraction (GIXD) were exploited with high precision diffract meters on rotating anode X-ray generators (SLX2000+UltraX, TTR-450, Rigaku Co.). Thin films on Si (100) were prepared by spin-coating method with acetone as a solvent. For cocoa butter, uniform layers were easily formed by annealing, yet dewetted layers are obtained for some oils even after the annealing. A strong surface-induced preferred orientation is shown for all the samples, indicating anisotropy in intermolecular interaction. Furthermore, a distinct transformation from a double-layer structure to a single-layer structure is observed. We consider that those structures might correspond to smectic phases of liquid crystals.

Keywords: X-ray diffraction, surface structure, oil

The formation of ice nanostructures on Cu(001)
Jia Mei Soon1, Masashi Nakamura2, Hiroto Tajiri1, Osami Sakata1,3
1Japan Synchrotron Radiation Research Institute (JASRI)/SPRING-8, 1-1-1 Koto, Sayo, Hyogo, 679-5165, Japan, 2Department of Applied Chemistry and Biotechnology, Faculty of Engineering, Chiba University, Inage-ku, Chiba 263-8522, Japan, 3JST-CREST, 5 Sanban-cho, Chiyoda-ku, Tokyo, 102-0075, Japan, E-mail: jamie@spring8.or.jp

Nucleation of water into ice is an important process in diversified fields ranging from atmospheric chemistry to astrophysics to biology. The hydrogen-bonded network of water is well-understood in homogeneous nucleation but the influence of the substrate in heterogeneous nucleation leaves a lot of open questions to be answered. How does the interaction of water with the substrate affect hydrogen-bonding? To understand this dynamic process, it is essential to study the nano-structure of ice nucleation on the substrate. In this work, we study the structure of water adsorbed on the Cu(001) at 25K by measuring its crystal truncation rods (CTR) using synchrotron-based surface X-ray diffraction (SRXD). The results are compared with water adsorption on Ni(111) to evaluate the substrate effect, whereby lateral relaxation and vertical buckling of the surface atoms are observed in order to accommodate the water in an atop position. We discuss the surface structural factors leading to this phenomenon. High photon intensity synchrotron-source x-ray at SPRING-8 provides accurate structural information of the weak interaction of molecules on surfaces even for a small molecule like water.

Keywords: surface X-ray diffraction, water nucleation, copper