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Observation on structure in the surface region of cocoa butter, POP, SOS and POS by X-ray diffraction

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Cocoa butter, prepared from ground roasted cacao beans, has six polymorphisms 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- stearoyl-2-oleoylglycerol), etc. Since there is some resemblance in molecular structure among them, POP, SOS and POS exhibit six or five polymorphisms 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

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The formation of ice nanostructures on Cu(001)

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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 homogenous 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 (SXRD). 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

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Structure determination of water chain adsorbed on Pt(211)

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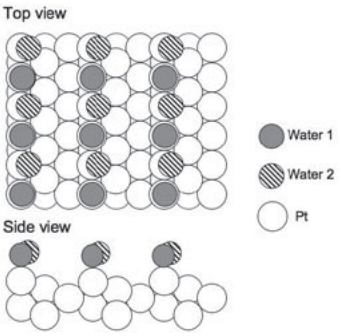
The interaction of water with metal surfaces is of considerable importance in many fields of science. Many studies have focused on the detailed structure of ice-like bilayer. [1] The low-dimensional structure of water on surface remains controversial. We determined the structure of water chain adsorbed on Pt(211) using surface x-ray diffraction (SXD). SXD measurement was performed with UHV chamber at BL13XU for surface and interface structure determination in SPring-8. Structural analysis demonstrates that water is molecularly adsorbed on the step of Pt(211) as shown in figure. Two different kinds of water are found at the top of the step. One is adsorbed on Pt (Water 1), and the other forms hydrogen bond with adsorbed water (Water 2). Pt - O length of adsorbed water is shorter than that on Pt(111), indicating that water binds strongly to the step Pt atom. This result is consistent with previous theoretical and experimental study. [2]



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Observation of 1D and 2D nanostructures using the X-ray reciprocal-lattice space imaging method

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