SHORT COMMUNICATION

Alkyl Chain Packing in a β' Triacylglycerol Measured by Atomic Force Microscopy

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The lateral packing of alkyl chains in single crystals of β' $C_{12}C_{14}C_{12}$ (β'-LML) was investigated by atomic force microscopy. The geometry of the methyl terrace fully supports the structure model proposed on the basis of X-ray diffraction data and symmetry considerations.

KEY WORDS: Atomic force microscopy, β', methyl terrace, triacylglycerol structure.

A crystallographic investigation of twinned crystals of the β' modification of the triacylglycerol LML ($C_{12}C_{14}C_{12}$) was reported recently (1). The unit cell dimensions of β' LML are a = 22.9 Å, b = 5.7 Å, c = 66.8 Å, α = 90°, β = 91° and γ = 90°. On the basis of unit cell dimensions, density and space group symmetry, it was concluded that the unit cell is a nearly orthorhombic flat box, containing eight LML molecules. Unit cell dimensions and symmetry elements further require that the alkyl chains make an angle of 25° with the c axis, and that the LML molecules are bent at the glycerol site. An X-ray powder diffraction study of compounds of selected different triacylglycerols showed that the LML molecules are most likely crystallized in a 1-2 configuration.

The proposed orientation of the alkyl chain subcells with respect to the unit cell axes of LML (1) is schematically shown in Figure 1. The positions of the alkyl chains at the corners and at the center of the $a_s b_s$ plane are given in Figure 1C.

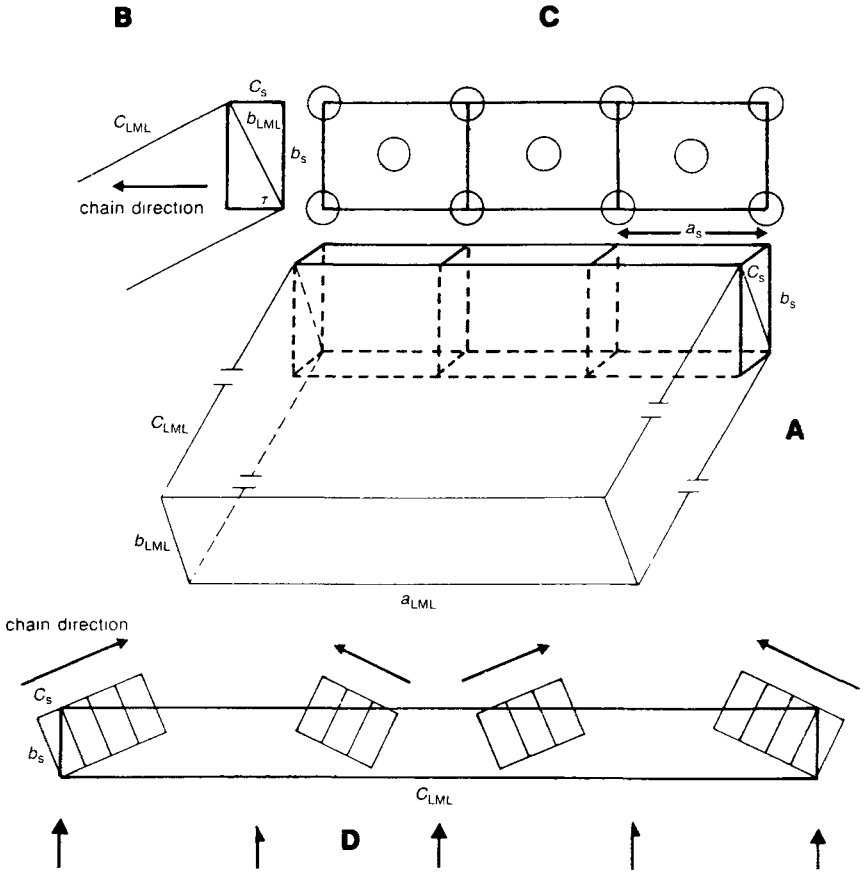

FIG. 1. Relation between the unit cell of β' LML and an O_1-like orthorhombic subcell. A, Three orthorhombic subcells drawn in the unit cell of β' LML; the a_s and a_{LML} axes coincide, whereas the $c_s$and the c_{LML} axes make an angle of 25° (90-τ). The b_{LML} axis coincides with the diagonal of the $b_s c_s$ plane. B, Projection of the *bc* plane, containing the *b* and *c* axes of both the subcell and the true LML unit cell. C, Projection of the $a_s b_s$ plane showing the positions of the alkyl chains, indicated by circles. D, Projection of the $b_{LML}c_{LML}$ ($\equiv b_s c_s$) plane schematically showing the relative positions of the subcells and the directions of the alkyl chains, which are parallel to c_s (ref. 1).

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Awaiting the result of a full X-ray structure determination, we now report the results of atomic force microscopy (AFM) visualizing the lateral packing of the alkyl chains at atomic resolution.

EXPERIMENTAL PROCEDURES

Twinned crystals of β' LML were grown as reported earlier (1). A TopoMetrix (Darmstadt, Germany) TMX 2000 Atomic Force/Lateral Force Microscope was used to probe the c surface structure of β' LML crystal. The AFM microscope was calibrated on a mica sample in the usual way. Three different positions at the crystal were probed, producing identical results.

RESULTS AND DISCUSSION

The orientation of the alkyl chains in the unit cell and the crystal habit dictate that the macroscopic crystal surface, which is perpendicular to the c axis (the $a_{LML}b_{LML}$ plane), consists of terminal methyl groups of LML molecules. The arrangement of the methyl groups in the crystal surface must therefore be as in Figure 1C, but now with mutual distances of $a_{LML}/3 = 0.76$ nm in the a direction and of $b_{LML} = 0.57$ nm in the b direction.

Figure 2 shows the surface structure of the macroscopic c plane of the crystal as measured by AFM. A projection of the structure is shown in Figure 3. Superimposed on this picture is a face-centered, rectangular 0.76 nm × 0.57

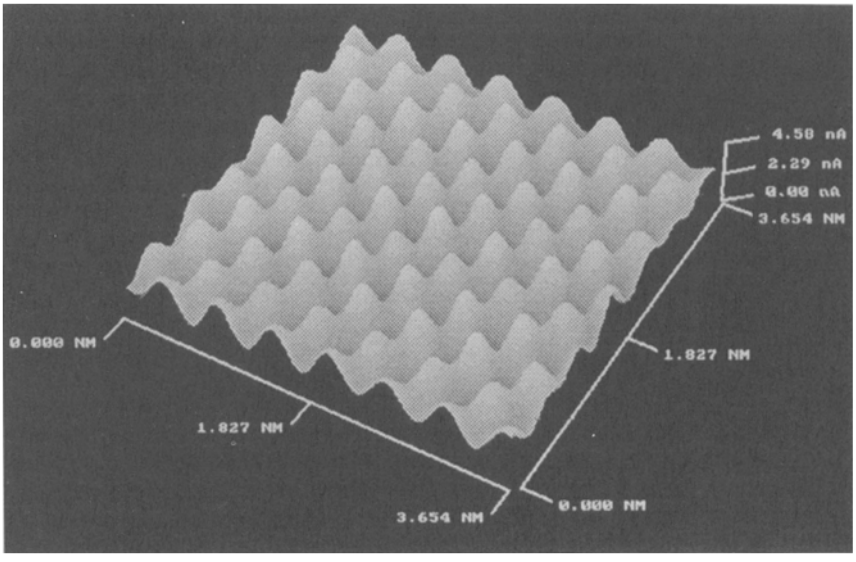

FIG. 2. The surface structure of the c plane of a β'-LML crystal, as measured by atomic force microscopy.

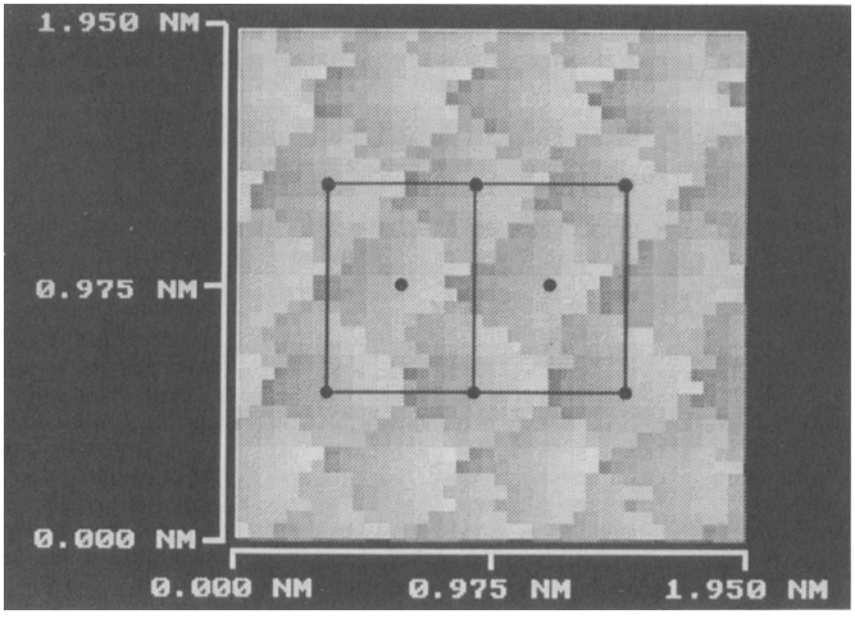

FIG. 3. Projection of the structure of the c plane of the β' LML with a face-centered 0.76 nm × 0.57 nm grid superimposed.

nm grid representing the theoretical positions of the alkyl chains (see Fig. 1C). The agreement between the AFM measurement of the surface structure and the theoretical geometry of the lateral arrangement of methyl groups in the crystal surface is remarkable. A complete X-ray structure determination of the β' LML structure is in progress.

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REFERENCE

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