

Disorder and Twinning: Equations and Applications to the Structure of the Carboxysome Shell

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Although crystal structure determination for proteins is sometimes routine, this is often not the case. Structure determination may be complicated by a number of factors, including certain kinds of crystal growth disorders, of which merohedral twinning is one particularly interesting type. Twinning can prevent successful structure determination if it goes undetected, but it is often treatable if it is correctly identified. The effects of twinning are sometimes masked by other phenomena, such as pseudo-centering, scattering anisotropy, and non-crystallographic symmetry. Recently developed intensity statistics equations for dealing with these complications will be discussed, along with the emerging structure of proteins from the carboxysome shell, determined from crystals suffering from merohedral twinning. The carboxysome is a polyhedral protein shell, which resembles a viral capsid and is found in many bacteria. Bacteria employ the carboxysome shell as a primitive organelle by enclosing RuBisCO and other enzymes in its interior, in order to carry out cellular CO₂ fixation in a sequestered environment. This work is supported by the NIH and the BER Office of the DOE.

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