

DATA VALIDATION OF MODULATED AND COMPOSITE STRUCTURES

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The lattice periodicity is considered essential for the characterization and comprehension of a crystal structure. A couple of decades ago, mineral calverite was found and baffled crystallographers since it did not obey the law of rational indices. These types of structures cannot be indexed using conventional three integer indices. Further analysis on such structures revealed that they deviate from the regular structures by having perturbations in their atomic position, occupation and/or thermal motion. These fluctuations can be described as a modulation wave, leading to the name modulated structures. The symmetry of the crystal structure can be described in the (3+d) super space using superspace group. In recent years, several of these types of structures attracted various scientists on account of their interesting physical properties. The number of modulated structures being published is increasing steadily indicating the need for a database to house them and describe them properly. The Powder Diffraction File is responding to this necessity of the scientific community by incorporating modulated structure starting with Release 2011. This poster will emphasize the data validation procedure implemented to evaluate modulated and composite structures before adding them to the database. A brief description of the editorial database changes required to house modulated structures will also be presented.