

Modulations in complex structures – two case studies

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There is something very appealing about rendering complex approximations to incommensurately modulated structures simple by using the super space formalism to present them in a clear and succinct form. There are however cases when the basic structure itself is quite complex, and this makes analysis a little more involved. First of all, the solution of the underlying parent structure is far from straight-forward, and secondly, the identification of the primary cause of the modulation is more difficult. We present here two cases that present such problems, the structures of $\text{ht-Sb}_2\text{Zn}_{3-x}$ and that of $\text{Ce}_{13}\text{Cd}_{58}$. The first structure belongs to a class of compounds that form between the zinc group metals and the pnictides. They typically consist of rigid pnictide frameworks and interstitial Zn and Cd, and the ordering of Zn/Cd forms complex commensurate superstructures. In the compound $\text{ht-Sb}_2\text{Zn}_{3-x}$ the Sb network is modulated due to a slight icosahedral mismatch, and the combination of the two effects leads to a very complex arrangement indeed. The second compound, $\text{Ce}_{13}\text{Cd}_{58}$ is a ortho-hexagonal approximant to the stable binary $\text{CaCd}_{5.7}$ type quasi crystals. Here the incommensuration is driven by two coupled mechanisms, the exchange of a Cd_2 dumbbell by a single Ce atom, and the ordered partial occupancy of Cd_8 cubes.