

MS25-O5 Z-module dislocations in complex intermetallic phases

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Several intermetallic phases have structures where the atoms are located on the sites of a \mathbb{Z}^d , i.e. at positions x_i that are linear integer combination of $N > d$ vectors e_k arithmetically independant, where d is the dimension of the physical space:

$$x_i = \text{Sum}_{k=1,N}(n_k^i e_k)$$

These structures are best analyzed as cuts of large periodic objects in a space of dimension $N > d$. These objects can carry high dimensionnal N -dim dislocations the Burgers vectors of which are linear integer combination of the basic vectors e_k .

We shall illustrate on simples examples the basic properties of these Z-module dislocations also designated by *metadislocations*, as a function of the relative values of the rank N of the module and the dimension d of the physical space. In particular, when Z-module superabundant, it is possible to build original dislocations the Burgers vector of which is entirely perpendicular to the physical space. These metadislocations are therefore insensitive to any stress fields and behave thus as "scalar" as we shall denominate them. These new defects will be exemplified in simple low dimensional cases.

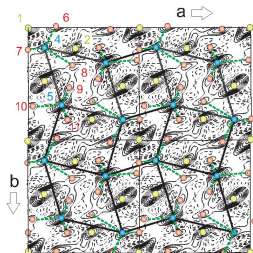


Figure 1. Z-projected charge density contour plot $\rho(x,y)$ of the approximant structure showing four unit cells. The Kepler tiling is indicated by the solid black lines.

Keywords: Oxide Quasicrystal, Approximant, Surface x-ray diffraction, Bariumtitanate

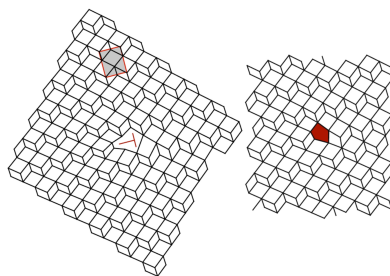


Figure 1. Example of a 2D periodic structure based on the \mathbb{Z}^3 : on the left a classical perfect dislocation; on the right, a so-called metadislocation (that is a perfect dislocation at 3D), boarding kind of a stacking fault.

Keywords: approximants, Z-modules, dislocations