MS29-P3 Estimation of the flip ratio from the diffraction pattern of 1D quasicrystal

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We estimate the number of phason flips randomly applied to atomic positions of the model 1D quasicrystal based on the Average Unit Cell concept within the statistical approach. Phasons can be understood in many different ways in terms of aperiodic crystals [1]. In this work we understand phasons as local rearrangements of structure units. They are known in literature as phason flips [2]. We use the Fibonacci chain built of long L and short S unit tiles as a model 1D quasicrystal. As a phason flips we consider LS→SL swap in the Fibonacci chain sequence. As a consequence of flip occurrence, the change in intensities of the diffraction peaks is observed. The standard correction to the intensity loss in calculated diffraction pattern during the structure refinement process is the Debye-Waller factor defined in perpendicular space.What we propose is to analyze phasons in the physical space using the statistical approach. Here, the atomic structure is modeled by a statistical distribution of atomic positions in physical space (so-called Average unit Cell concept [3-5]). Each single flip of the unit tiles influences the distribution, respectively for different structures. The deviation from the ideal distribution, where no phasons flips are applied, can be easily designated and by that the number of flips can be quantified.In order to retrieve the number of flips we develop yet more precise analysis, which is based on power series expansion of the characteristic function for statistical distribution. This characteristic function for quasicrystals is the structure factor expressed within statistical approach. The moments of the distribution are fitted against diffraction (reference) data. It can be shown that the value of second moment gives full information about the number of flips. This statement is based on the relation between moment value and flip ratio α, which can be calculated analytically. Higher-order moments tend to differ from the theoretically derived curve (Fig. 1).

References

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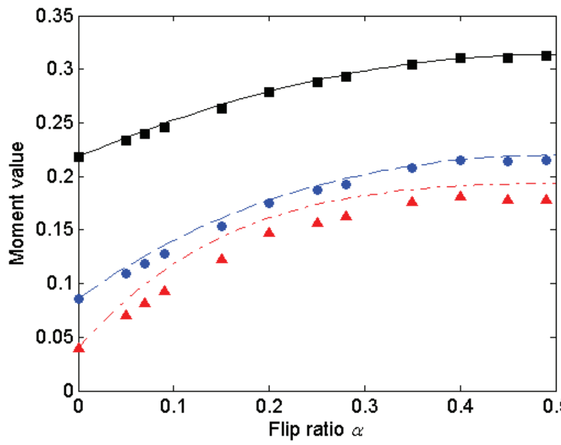

Figure 1. The values of the second- (black square), fourth- (blue circle) and sixth moment (red triangle) fitted with respect to the flip ratio α. The deviation from the theoretical curve (solid, dashed, dash-dotted respectively) is observable for higher-order moments

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