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Abstract

The diffraction pattern of a model disordered structure has been thoroughly analysed. The structure is based on a crystal lattice and by varying certain set of parameters it is possible to obtain a smooth transition from a perfect crystal to an amorphous state. The lattice distortion as well as a range of the coherent scattering may also be easily controlled, so it is possible to observe an influence of the short-range order as well as its relation to the range of the coherent scattering, on the diffraction pattern.

Introduction

A diffraction pattern of any structure can be obtained by the Fourier transformation of its atomic positions. The classical crystallographic approach, however, is based on the concept of an unit cell and reciprocal lattice, therefore its validity is constrained to the analysis of perfectly periodic crystals. If a given structure is not of this type, the unit cell does not exist and this approach fails. In the case of modulated structures, one can recover the unit cell and periodicity by means of the high-dimension analysis. [1] Nevertheless, this method is not applicable to the other types of structures. It has been shown however [2], that the diffraction pattern of such aperiodic structures may be correctly described in the average unit cell approach based on the reference lattice concept. In this approach a periodicity of the real structure is not important, yet when it holds, the average unit cell becomes a classic unit cell. It is possible to construct probability distributions of positions of atoms (nodes) relative to the unit cell and then calculate Fourier transformation to get so-called envelope function, which correctly describes intensities for certain set of the well-defined scattering vectors.[3]

In the case of a complete lack of the long-range order, only the continuous part of the diffraction pattern is observed, whereas for an ideal long-range order only the Bragg peaks remain. The diffraction image of any disordered structure, exhibiting a short-range order, may consist of these two parts scaling differently with a number of atoms N : a set of Bragg peaks which scales as N^2 and a continuous part scaling linearly with N (and a background but not taken into account here) what makes an interpretation of the pattern very difficult. A shape of such diffraction pattern depends on many different factors. On one hand, a diffraction pattern is strictly connected with the structure itself, in particular any (whether long or short-range) order is usually reflected in the diffraction peaks. On the other hand though, characteristics of a radiation used to perform given diffraction experiment is also extremely important. A range of the coherent scattering can be of the utmost importance in an analysis of any diffraction pattern. In the same manner, one can take into account the influence of the size of seeds in the case of powder diffraction.

The scope of this work was to observe the influence of the short-range order and its relation to the range of the coherent scattering on the diffraction pattern. Changes in the shape of diffraction peaks as a function of

some parameters have also been investigated. There are several well-defined extreme cases, what proved to be very helpful and allowed to control the validity of the calculations. Between these extremes exists a large variety of disordered structures and changes in the diffraction pattern can be observed.

Model description and results

The model structure in its one-dimensional case is based on an infinite periodic chain with the unit cell of a length equal to a , which was also taken as a unit of length. In the two-dimensional case, the base structure is a square lattice. Taking the chosen node as the center of the structure (node number zero), one superimposes a Gaussian shift on the remaining nodes. Consequently, every node is shifted from its original position by a random factor ε with the standard deviation σ . One can therefore describe the position of every node as $x(n) = n \cdot a + \varepsilon(n)$, where n is the node number, a - the original unit cell length and $\varepsilon(n)$ - the Gaussian shift with the standard deviation σ .

To simulate vanishing correlations between distant nodes, the standard deviation σ has been set to increase linearly with the node number n , that is $\sigma(n) = \sigma_0 + |n| \cdot \Delta\sigma$, where σ_0 and $\Delta\sigma$ are arbitrary chosen positive constants. Such dependency preserves the short-range order but makes the correlations vanish with distance. Assuming $\Delta\sigma = 0$ and $\sigma_0 > 0$ the well-known Debye-Waller factor describing the thermal motions of the atoms can be reproduced (for appropriately small σ_0 values relative to the unit cell length). By setting both parameters to zero, one gets a periodic crystal. The parameter σ_0 has been put to zero as it is not very interesting here. The parameter $\Delta\sigma$ is responsible for the strength of correlations between nodes positions and effectively controls a range of the structural order. Moreover, to reflect a finite range of the coherent scattering, instead of taking into consideration the entire, infinite chain, only finite clusters of given size N have been taken for further calculations. To get rid of fluctuations coming from the random factors the calculations have been performed for a big number of separate clusters and then average values have been obtained. Both full diffraction patterns coming directly from nodes positions and envelope functions obtained within the average unit cell approach (as a square of the module of the Fourier transform of probability distributions created for the chosen scattering vectors) have been calculated. In the selected points the envelope function is accurate and shows correct values of intensities. The continuous part as well as the Bragg peaks can be easily distinguished (fig.1).

[Insert fig.1 about here]

Changes in height and width of peaks have been also investigated. One can expect that peaks should on one hand narrow with rising N because more atoms will then take part in the diffraction but on the other hand should broaden due to $\Delta\sigma$ parameter and vanishing correlations. It turns out that these two competitive effects give as a result constant peak width (fig. 2).

[Insert fig.2 about here]

As expected, for strong short-range order regime, diffraction peaks are scaling nearly as N^2 , i.e. these are the Bragg peaks what is visible as a linear function on the initial fragments of characteristics shown on fig.3 (the main plot). Beyond this range, scaling of the peaks changes and eventually decays becoming a part of the continuous part of the diffraction pattern what is clearly visible from the linear function with

[Insert fig.3 about here]

The maximum of the peak height (the main plot on the fig. 3) has been further investigated. The results for the first and second peak turned out to be identical, only parallel shift on the double logarithmic scale is needed. The position of this maximum for each peak is proportional to $(\Delta\sigma)^{-1}$ (fig.4).

[Insert fig.4 about here]

For given large N (here equal to 201) also the height of peaks as a function of $\Delta\sigma$ has been analysed. (fig. 5). It turns out that this height is proportional to $(\Delta\sigma)^{-2}$.

[Insert fig.5 about here]

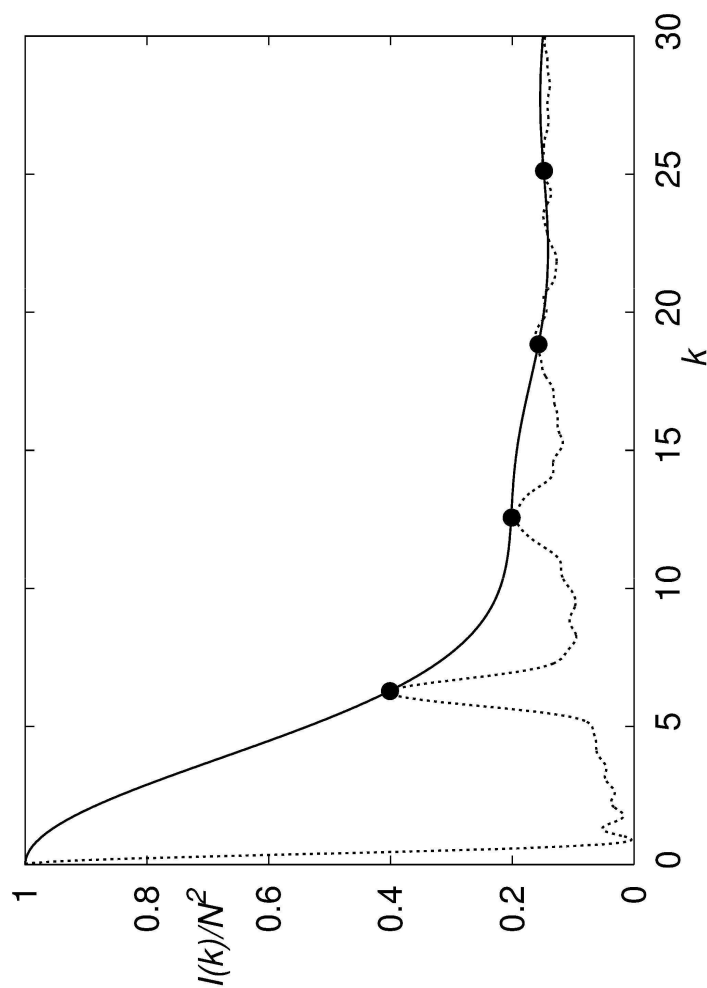
The average Patterson functions also have been calculated. This function is obtained by the reduction of the Patterson function, which is basically the inverse Fourier transform of the diffraction pattern, to the average unit cell. As a result, one can conclude that these functions are quite indistinctive as long as the range of coherent scattering multiplied by $\Delta\sigma$ remains constant (fig.6).

[Insert fig.6 about here]

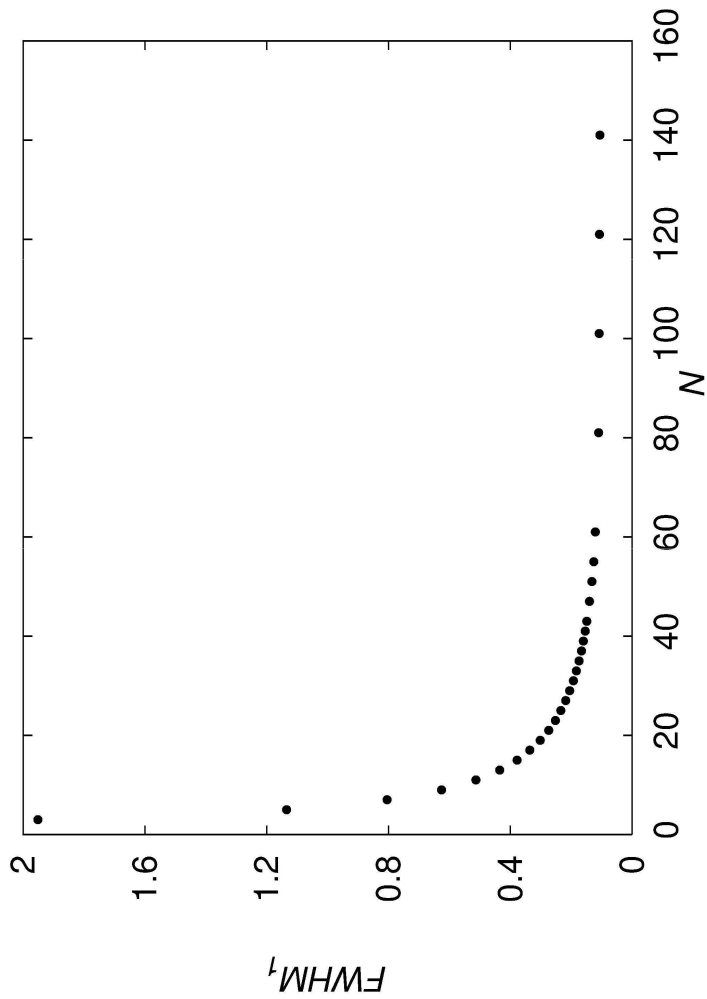
Conclusions

In this paper we have shown that calculated in the average unit cell approach envelope functions correctly describe a diffraction pattern consisting of different parts: Bragg reflections (atomic part) and diffuse scattering (continuous part). An application of such statistical method makes possible to fit to the real diffraction pattern an appropriate distribution function with only a few adjustable parameters. Shapes of peaks as a function of the range of correlations and coherent scattering have also been investigated.

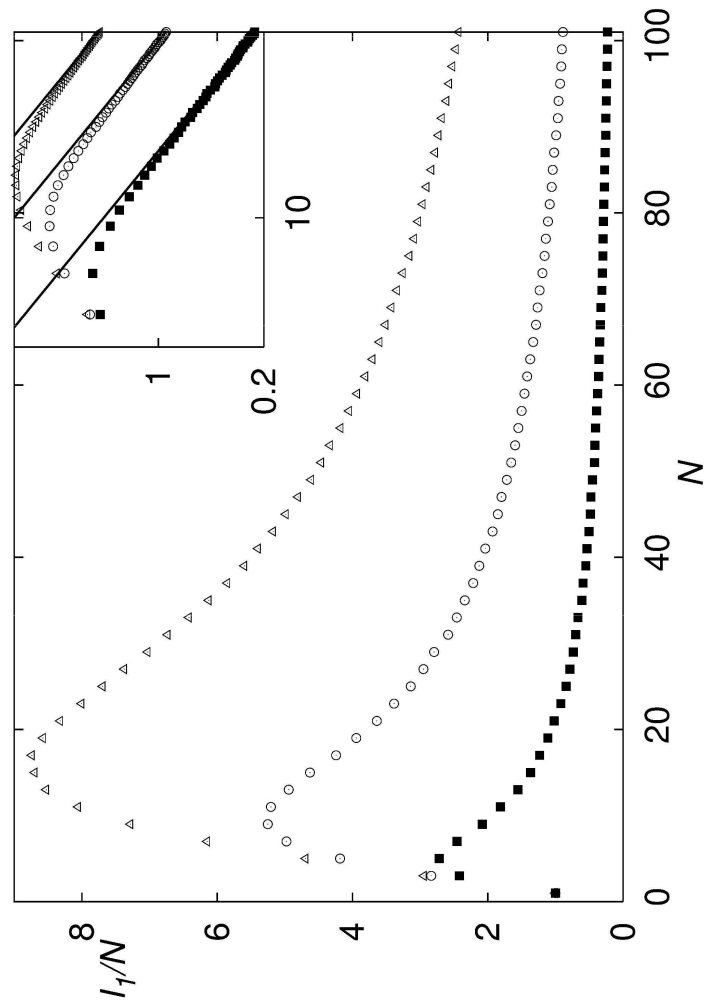
The correctness of all calculations is ensured by the extreme cases with well-known solutions. In one case, by setting both range of correlations and range of coherent scattering as effectively infinite, one obtains the pattern of perfect, infinite crystal, that is a set of infinitely narrow Bragg peaks. On the other end of the spectrum there is a completely disordered random structure with the diffraction pattern consisting of the continuous part only.



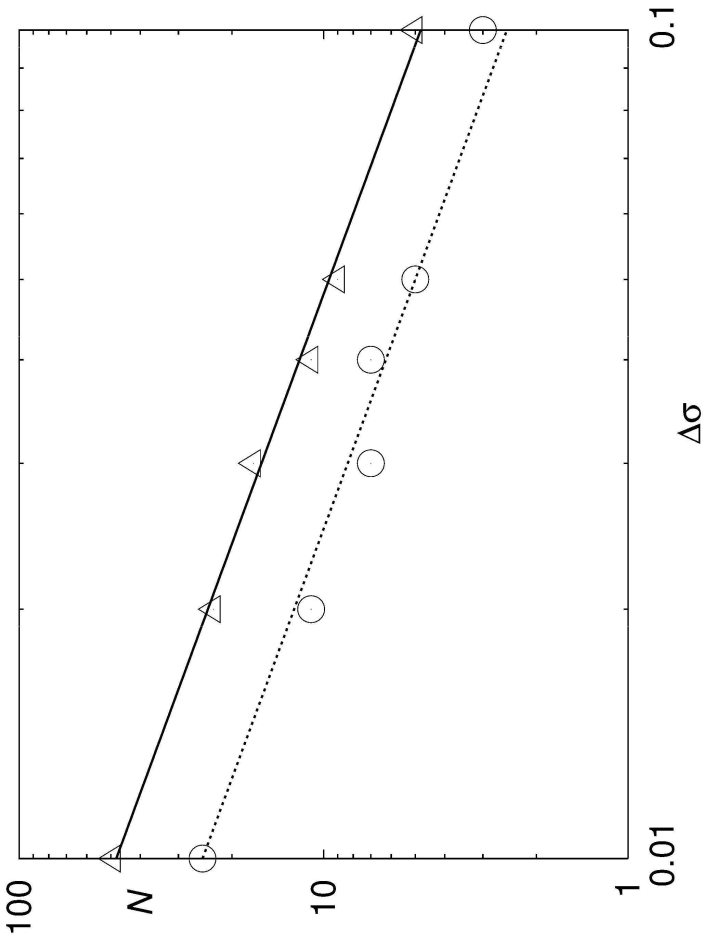
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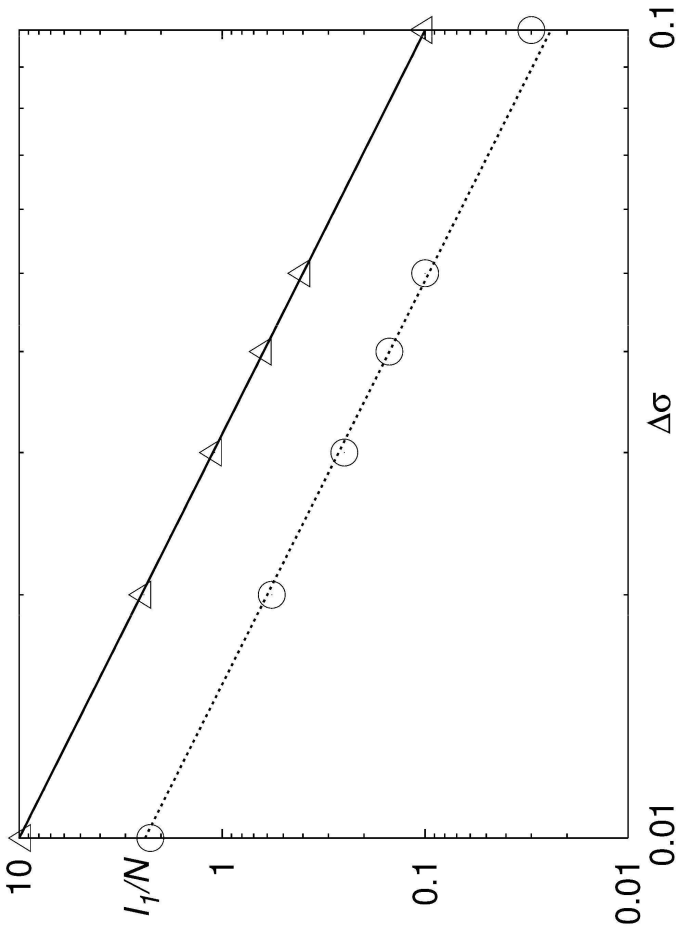
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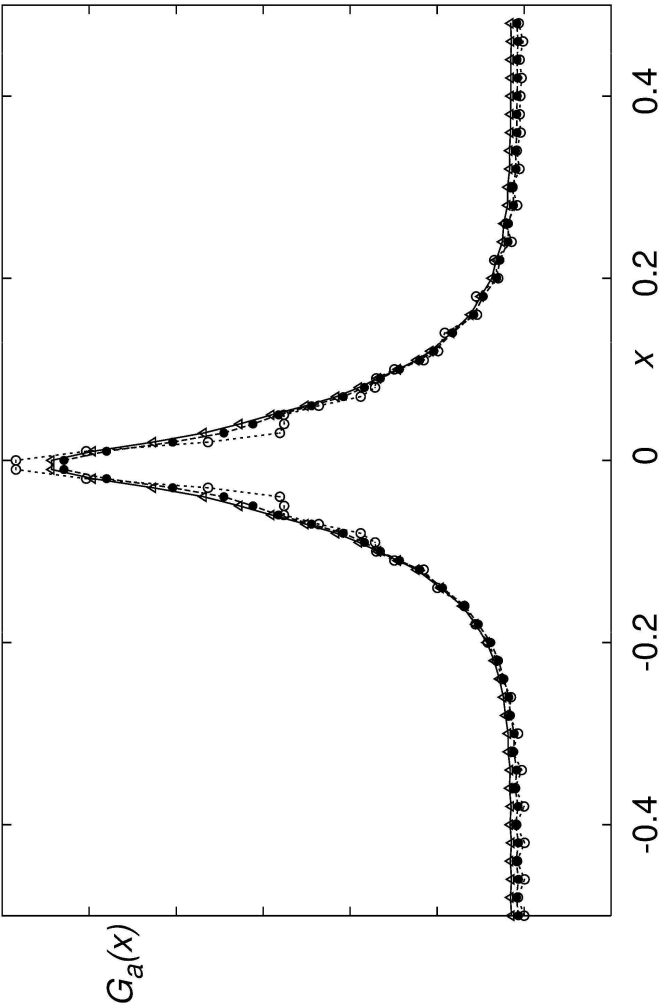
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