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**Robust, automated detection of defects in direct images of periodic structures**

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We present a novel algorithm for robust, automated detection of point defects, dislocations, and other defects in direct microscopic images of periodic structures like crystal lattices [1,2], graphene layers [3], or biological membranes [4]. The algorithm accepts images registered by a number of microscopic imaging techniques, including SEM, TEM, HRTEM, STEM, Z-contrast, and AFM. The only constraint imposed on image acquisition method is that all visible primitive cells of the lattice are of almost identical dimensions. Small rotations, translations and scalings of particular cells are acceptable and are not treated as defects, so there is no need to “unbend” the structure [5] or to remove spherical aberration of the apparatus [6]. Also, to obtain correct results the contrast transfer function does not need to be corrected [7] and no background normalization is necessary.

The first step of the algorithm is to determine lattice spatial dimensions in pixels by means of a procedure imported from the *2dx* package [4]; this procedure performs analysis of peaks in the power spectrum of numerical diffractogram of the input image *i*. Once the unit cell size is known, a few cells are randomly selected, and for each cell its clockwise and counterclockwise rotations are computed. Then, for each rotated and unrotated pattern several upscaled and downscaled patterns are calculated. For every pattern *p* obtained in this way the map of statistical correlation coefficient $\rho_p(x,y)=cov(p,i_{x,y})/(var(p)var(i_{x,y}))^{1/2}$ is computed, where $i_{x,y}$ is a subimage of *i* located at *(x,y)* and of size matching that of *p*. This coefficient is invariant under affine remappings of gray levels of *p* and *i*; it has been proven to be a robust measure in pattern matching [8] and can be efficiently computed using the fast Fourier transform and the running sums algorithm [9]. Next, step all maps $\rho_p$ coming from rotated patterns *p* are derotated to unify coordinates; there is no need to account for scaling at this step. Then, a list *L* of all local maxima in all maps $\rho_p$ is created. Each element of *L* is inspected by a classifier deciding its correspondce to a true cell of the lattice. Once locations of all defect-free lattice nodes are known, for every node its neighborhood is determined. We obtain an adjacency graph whose vertices are labeled with spatial positions of lattice nodes. This graph is used to find crystallographic defects: vacancies and voids, interstitial defects, Frenkel pairs, edge dislocations, distinct impurities and clusters of these, or Stone-Wales defects. The final result is an image in which all defects are drawn and labeled. In future the algorithm can be extended to produce LaTeX-formatted output in the Kröger–Vink notation for point defects.

The algorithm proved robust, fast, and efficient in automatic localization of defects when tested on images of graphene layers, crystal lattices, and biological membranes; all defects have been localized successfully. It can be easily incorporated into public-domain open-source software packages for crystallographic analysis, especially in the quality assurance domain.

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**Novel Combination of 3DXRD and Grain Boundary Tracking for Mapping Polycrystaline Al-alloys**

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A novel method that can provide accurate analysis of individual grains has been produced by combining X-Ray Diffraction (XRD) microscopy with grain boundary tracking (GBT) [1]. Since XRD is a non-destructive technique for characterizing bulk materials, *in-situ* analysis of metals can be performed both with and without applied loads. Loads can also be applied close to the point of fracture whilst still producing practical data. This combination of techniques, known as GBTXRD, provides accurate information about individual grain orientations from near field XRD analysis, whilst the grain boundary tracking accesses 1 micron level analysis of grain morphologies. The experiments used to derive GBTXRD analysis, further developments and possible applications, shall be presented.

An X-ray pencil beam was employed to perform the analysis of two types of materials: Al single crystal wire and Al-4mass%Pb alloy. The single crystal wire was used for alignment purposes and to determine a relationship between the wire’s diameter and the diffraction spots it produced. However, relationships generated employing the data obtained from the single crystal wire were ambiguous; this was believed to be due to extinction factors. A preliminary 3-dimensional X-Ray diffraction (3DXRD) grain map of the Al-alloy was produced at the European Synchrotron Radiation Facility (ESRF) [2], after which XRD and computer tomography (CT) was carried out at Spring-8 Synchrotron in Japan. The 3DXRD grain map was used to determine the orientation of the grains so that their respective diffraction spots could be located. The morphology of the grains were then determined from CT images of the sample subjected to a liquid metal wetting method using Ga. These CT images were exploited for grain boundary tracking, which provided a more accurate description of the position and morphology of the grains than can be achieved through 3DXRD. Upon determining which diffraction spots were related to which grain, analysis of the relationship between various parameters describing both the grain and its relevant diffraction spots were determined. Correlation coefficients where calculated for all the groupings of these parameters. By combining results from the parameters with the three best correlation coefficients using the data acquired at Spring-8, it was possible to describe the grain misorientation with an accuracy of 100%.

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**Masquerade: Improving Data Quality with Masks for Beryllium Rings**

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