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1 Article

# 2 The effect of crystal defects on 3D high resolution 3 diffraction peaks: a FFT-based method

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13 **Abstract:** Forward modeling of diffraction peaks is a potential way to compare the results of  
14 theoretical mechanical simulations and experimental X-Ray Diffraction data recorded during in situ  
15 experiments. As the input data are the strain or displacement field within a representative volume  
16 of the material containing dislocations, a computer-aided efficient and accurate method to generate  
17 these fields is necessary. With this aim, a current and promising numerical method is based on the  
18 use of the Fast Fourier Transform (FFT) method. However, classic FFT-based methods present some  
19 numerical artifacts due to the Gibbs phenomenon or “aliasing” and to “voxelization” effects. Here,  
20 we propose several improvements: first, a consistent discrete Green operator to remove “aliasing”  
21 effects and second, a method to minimize the voxelization artifacts generated by dislocation loops  
22 inclined with respect to the computational grid. Then we then show the effect of these  
23 improvements on theoretical diffraction peaks.

24 **Keywords:** Dislocations; diffraction; FFT-based method; Discrete Green operator; voxelization  
25 artifacts; sub-voxel method; simulated diffraction peaks; scattered Intensity

26

## 27 1. Introduction

28 X-Ray diffraction is one of the most powerful non-destructive tools to investigate materials, as  
29 their wavelength is commensurate with the distance between atoms within a crystal [1–9]. Successive  
30 improvements of both the X-Ray sources (from X-Ray tubes to third generation synchrotrons) and  
31 detectors (from photographic plates and gas counters to fast two-dimensional arrays) have led to a  
32 tremendous increase in the quantity of data recorded per unit time, allowing real time *in situ* or *in*  
33 *operando* measurements [10,11]. It is now possible to determine the 3D grain microstructure of a bulk  
34 material with a submicron resolution (using Topo-Tomography), to follow the evolution of the elastic  
35 strain state of the grains of a polycrystal during mechanical tests (3D-XRD, far field diffractometry),  
36 or to measure the distribution of strains within a few grains in real time (2D diffractometry)  
37 [12,13]. Such experiments result in terabytes of data recorded within a few days, which need to be  
38 efficiently analyzed. In fact, only a low fraction of those data is actually treated because scientists lack  
39 both time and software for further analysis [14].

40 The classical techniques used to analyze the 1D or 2D diffraction patterns recorded during tests  
41 performed on polycrystalline specimens such as the Rietveld method, the square sines method to  
42 measure internal stresses, or CMWP fitting for dislocations content often rely on simplified and  
43 mathematically tractable models of a microstructure. Calculations which may involve simplifying  
44 hypothesis lead to a general formula which can be used to fit one or several parameters of the

45 microstructure (dislocation densities and type, internal stress tensor...) to the diffraction pattern  
46 (peak profiles, variation of the  $2\theta_B$  angle with orientation...)

47 During the last ten years, several authors proposed the opposite approach: forward modeling  
48 [15–22]. This requires the design of a microstructure and the simulation of its behavior (often under  
49 process or thermo-mechanical solicitation), the computation of the elastic strain field or the  
50 displacement field. The last step is the generation through a ‘virtual diffractometer’ of a theoretical  
51 diffraction pattern (different  $\mathbf{G}$  vectors and different orientations of the lattice planes), which can be  
52 compared with the experimental one. Depending on the size of the simulated representative  
53 volume of matter and the experimental conditions such as the X-Ray beam coherence, different  
54 assumptions can be done such as a coherent beam (where the amplitudes scattered by different points  
55 add) or an incoherent beam (scattered intensities add), or for a partially coherent beam where a full  
56 calculation may be necessary. Such modeling can be quite successful and can be used to validate the  
57 different steps involved, mainly the microstructure and the constitutive law used to simulate the  
58 material’s behavior.

59 However, as diffraction peaks contain information on different scales of a specimen: from  
60 average quantities such as Type I (average) stresses related to the peaks’ positions, Type II (at grain  
61 level) stresses related to its width, and Type III stresses (near the core of defects such as dislocations)  
62 related to the peaks’ tails, a realistic simulation of a diffraction peak requires a description of a  
63 material’s Representative Volume Element with a very fine mesh, i.e. a huge amount of CPU time  
64 with classical methods used for simulations such as the Finite Element Method.

65 Numerical approaches based on the FFT for calculating the stress and strain fields within a  
66 composite material received a surge of interest since the pioneering work of Moulinec and Suquet  
67 [23,24]. They were first developed to compute effective properties and mechanical field of linear  
68 elastic composites[23–26] and were extended to heterogeneous materials with eigenstrains  
69 (dislocations, thermal strains...) [14,27–30]. They are also used for conductivity problems [31], non-  
70 linear materials [25,27], viscoplastic or elastoviscoplastic polycrystals [32–36]. Today, FFT based  
71 approaches represent alternative to finite element method because they are rather attractive in terms  
72 of computation time [32].

73 However initial tests indicate that the displacement field computed (essential for diffraction  
74 pattern generation) with FFT algorithms presents some numerical artifacts. These numerical artifacts  
75 are due to Gibbs phenomenon or “aliasing” and to voxelization. The accuracy of the calculated strain  
76 or displacement field is strongly influenced by these shortcomings and the simulated peaks may  
77 provide wrong information on mechanical behavior or material characteristics. Therefore, it is  
78 important to control these artifacts to simulate correct diffraction pattern in the case of a  
79 microstructure containing different phases, grains, and crystal defects.

80 The aim of this paper is to improve the accuracy of the displacement field for diffraction peak  
81 generation. This improvement is based on the introduction of a consistent discrete periodized Green  
82 operator associated with the displacement field in order to take explicitly into account the  
83 discreteness of the discrete Fourier Transform method [37]. The improvement of the voxelization in  
84 FFT-method is performed through a sub-voxelization method will be described for inclined  
85 dislocation loops. These improvements are reported and discussed. In the section 2, the FFT-based  
86 method to compute the displacement field in a periodic medium is described. In section 3, the  
87 treatment of voxelization problems in FFT-based approaches by a sub-voxelization method is  
88 detailed in the case of slip plane not conforming to FFT grid. In the section 4, simulation of diffraction  
89 peaks is reported and discussed.

## 90 2. Displacement field

### 91 2.1. FFT-based algorithm and mechanical fields

92 Let us consider a homogeneous elastic medium with eigenstrain assuming a periodic unit cell  
93 discretized in  $N \times N \times N$  voxels and subjected to an uniform overall strain tensor denoted  $\mathbf{E}$ . Here,  
94 this overall strain is the spatial average of the strain field in the unit cell (with external loading and a

95 given eigenstrain field). The unit cell contains dislocations (line defects) which are modeled with an  
 96 eigenstrain tensor. These dislocations create a displacement field during their motion along various  
 97 slip systems and thus generates strain/stress field [38].

98 The displacement vector is denoted  $\mathbf{u}$  and in the forthcoming equations,  $\mathbf{x}$  denotes any  
 99 position vector within the unit cell. All vectorial and tensorial fields will be written using bold  
 100 characters.

101 Starting from the equation for mechanical equilibrium,  $\text{div } \boldsymbol{\sigma}(\mathbf{x}) = 0$ , and using elastic  
 102 equations, the displacement field is given at every positions by [39]:

$$103 \quad \mathbf{u}(\mathbf{x}) = (\mathbf{B} * \mathbf{c}^0 : \boldsymbol{\varepsilon}^*)(\mathbf{x}) \quad (1)$$

104 Where the symbol  $*$  denotes the spatial convolution product,  $\mathbf{c}^0$  is the homogeneous linear elastic  
 105 stiffness,  $\boldsymbol{\varepsilon}^*$  is the eigenstrain field and  $\mathbf{B}$  is a third order Green operator defined in Fourier space  
 106 as:

$$107 \quad \widehat{B}_{ijk}(\boldsymbol{\xi}) = \frac{i}{2} (\widehat{G}_{ij} \xi_k + \widehat{G}_{ik} \xi_j) \quad (2)$$

108 in which  $\widehat{\mathbf{B}}$  is the Fourier transform of  $\mathbf{B}$  and  $\widehat{\mathbf{G}}$  is the Fourier transform of the elastic Green  
 109 tensor [39]. Therefore, using the Fourier transform of spatial convolution product, Equation (1) can  
 110 be written in Fourier space as:

$$111 \quad \widehat{\mathbf{u}}(\boldsymbol{\xi}) = \widehat{\mathbf{B}}(\boldsymbol{\xi}) : \mathbf{c}^0 : \widehat{\boldsymbol{\varepsilon}}^*(\boldsymbol{\xi}) \quad (3)$$

112 Several numerical results showed that the use of the third order operator  $\widehat{\mathbf{B}}$  derived from the  
 113 classic Green  $\widehat{\mathbf{G}}$  leads to spurious oscillations on the computed displacement field near materials  
 114 discontinuities. The Discrete Fourier transform (DFT) used in this algorithm indeed transforms a  
 115 periodic function in real space into a periodic function in reciprocal space. However, the operator  $\widehat{\mathbf{B}}$   
 116 commonly used is the continuous analytic operator truncated to the size of the unit cell of the  
 117 reciprocal space: it is not periodic function. To fix this problem, we a periodized consistent discrete  
 118 Green operator using the DFT. The Fourier transform of this new operator  $\widehat{\mathbf{B}}'$  is written as function  
 119 of  $\widehat{\mathbf{B}}$  (the mathematical details about its derivation are given in [37]) and reads:

$$120 \quad \widehat{\mathbf{B}}'(\xi_{ijk}) = A_{ijk} \sum_{m,n,p=-\infty}^{+\infty} \frac{(-1)^{m+n+p}}{(mN+i)} \frac{1}{(nN+j)} \frac{1}{(pN+k)} \widehat{\mathbf{B}}(\xi_{mN+i, nN+j, pN+k})$$

$$121 \quad \text{With} \quad A_{ijk} = \left(\frac{N}{\pi}\right)^3 \sin\left(\frac{i\pi}{N}\right) \sin\left(\frac{j\pi}{N}\right) \sin\left(\frac{k\pi}{N}\right) \quad (4)$$

122 Discrete frequency appearing in this equation is given when N is even by (T is the unit cell period):

$$123 \quad \boldsymbol{\xi} = \left(-\frac{N}{2} + 1\right) \frac{1}{T}, \left(-\frac{N}{2} + 2\right) \frac{1}{T}, \dots, -\frac{1}{T}, 0, \frac{1}{T}, \dots, \left(\frac{N}{2} - 1\right) \frac{1}{T}, \left(\frac{N}{2}\right) \frac{1}{T}$$

124 Here the sum on the  $\widehat{\mathbf{B}}$  operator is extended to the whole reciprocal space (in practice for  $m, n, p$   
 125 up to a few tens) and folded up onto the unit cell of the DFT with suitable coefficients. The inverse  
 126 transform of  $\widehat{\mathbf{u}}(\boldsymbol{\xi})$  gives the displacement field at the center of each voxel.

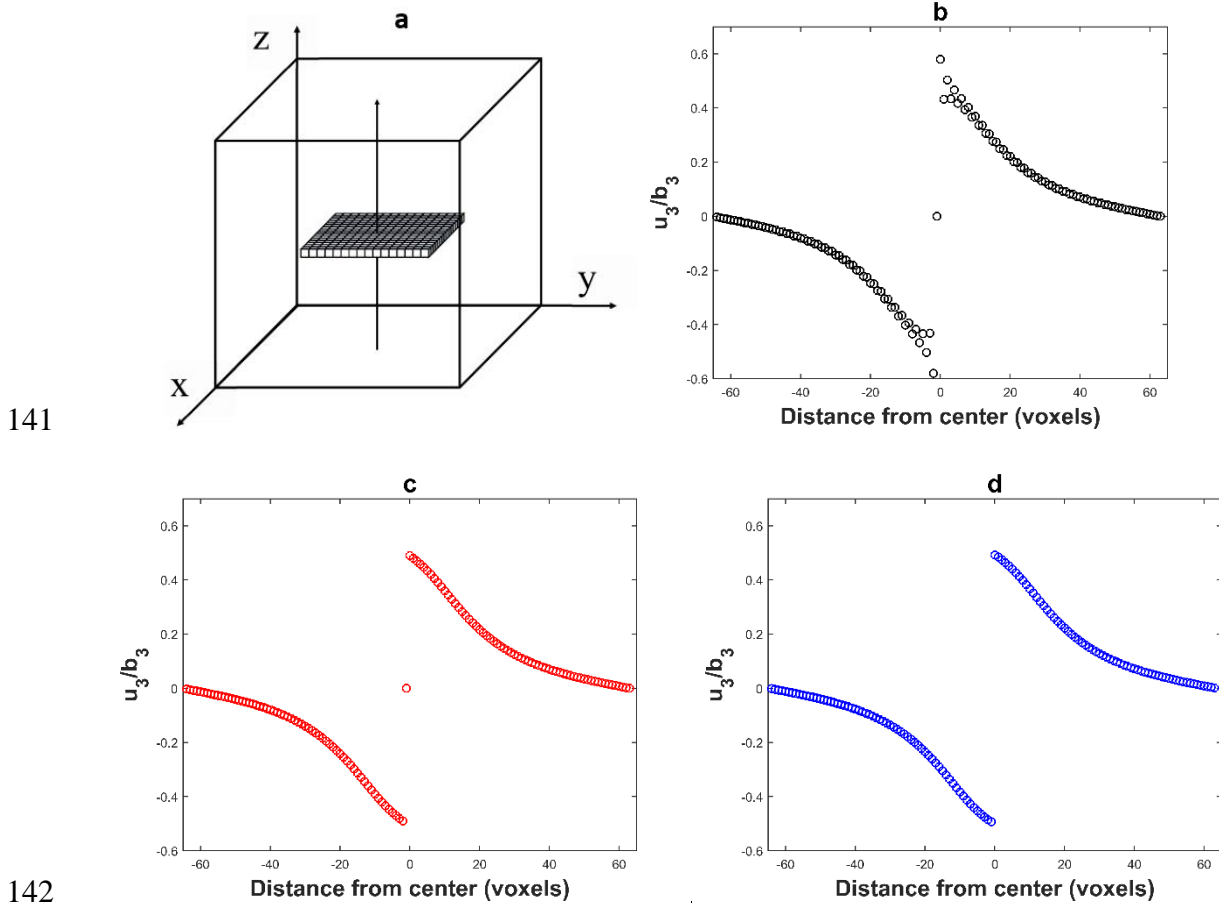
127 We can also compute the displacement field at each voxel's corner with a shifted operator using the  
 128 shift theorem:

$$129 \quad \widehat{\mathbf{B}}''(\xi_{ijk}) = A_{ijk} e^{p\pi \frac{i+j+k}{N}} \sum_{m,n,p=-\infty}^{+\infty} \frac{1}{(mN+i)} \frac{1}{(nN+j)} \frac{1}{(pN+k)} \widehat{\mathbf{B}}(\xi_{mN+i, nN+j, pN+k}) \quad (5)$$

## 130 2.2. Numerical examples

131 Let us consider a homogeneous material with isotropic elastic constant: Young's modulus  $E =$   
 132  $333.4 \text{ GPa}$  and the Poisson ration  $\nu = 0.26$ . This approximately corresponds to the room  
 133 temperature elastic constants of single crystalline Ni-based Superalloys. The unit cell (Figure 1a) is  
 134 discretized in  $128 \times 128 \times 128$  voxels and contains a square-shaped inclusion discretized in

135  $32 \times 32 \times 1$  voxels corresponding to an Eshelby-like square prismatic loop perpendicular to the z-  
 136 axis. In order to generate a shift of the upper surface of the inclusion relative to its lower surface by a  
 137 Burgers vector  $\mathbf{b}(0, 0, b_3)$  the voxels within the inclusion are submitted to an eigenstrain:  $\epsilon_{ij}^* = 0$   
 138 except  $\epsilon_{33}^* = 1$ . We thus have  $b_3 = t \times \epsilon_{33}^*$  where  $t$  the thickness of the inclusion in the z-  
 139 direction (i.e. the voxel size). This displacement field computed with the FFT algorithm using the  
 140 different periodized discrete Green operators is represented along z-axis in figure 1.



**Figure 1:** (a) Simulation of a squared dislocation in plane (001) by a platelet with eigenstrain; (b) Component  $u_3$  of the displacement field (normalized by  $b_3$ ) along the z axis (arrow) computed with the Green operator  $\mathbf{B}$  and showing oscillations; (c) Same component correct  $u_3$  computed with  $\mathbf{B}'$ . The displacement at voxel (64,64,64) is zero in the center of the inclusion (c) and  $b_3/2$  on its surface (c). (d) Same component correct  $u_3$  computed with  $\mathbf{B}''$ .

148 When computed along a line crossing a dislocation loop, the displacement field exhibits a  
 149 discontinuity with a jump equal to Burgers vector  $\mathbf{b}$ . This is indeed observed in figure 1. However,  
 150 the displacement field computed with the usual Green operator  $\mathbf{B}$  (figure 1b) also shows oscillations,  
 151 while which are not observed with the periodized operators  $\mathbf{B}'$  and  $\mathbf{B}''$ . An artificial damping of the  
 152 oscillations in figure 1b (such as a low pass filtering) might smooth these oscillations, but it would  
 153 also smooth the discontinuity.

### 154 2.3. Voxelization effect on the displacement field.

155 While the displacement field computed for dislocation loops having their planes parallel to the  
 156 faces of the simulated volume, artifacts appear for inclined loops, as shown in figure 2 for a  
 157 dislocation loop with a  $[0\bar{1}1]$  Burgers vector lying in a (111) slip plane of a fcc crystal. The  
 158 eigenstrain tensor is constrained in the region occupied by the dislocation loop (transformed voxels)  
 159 and is given by:

160

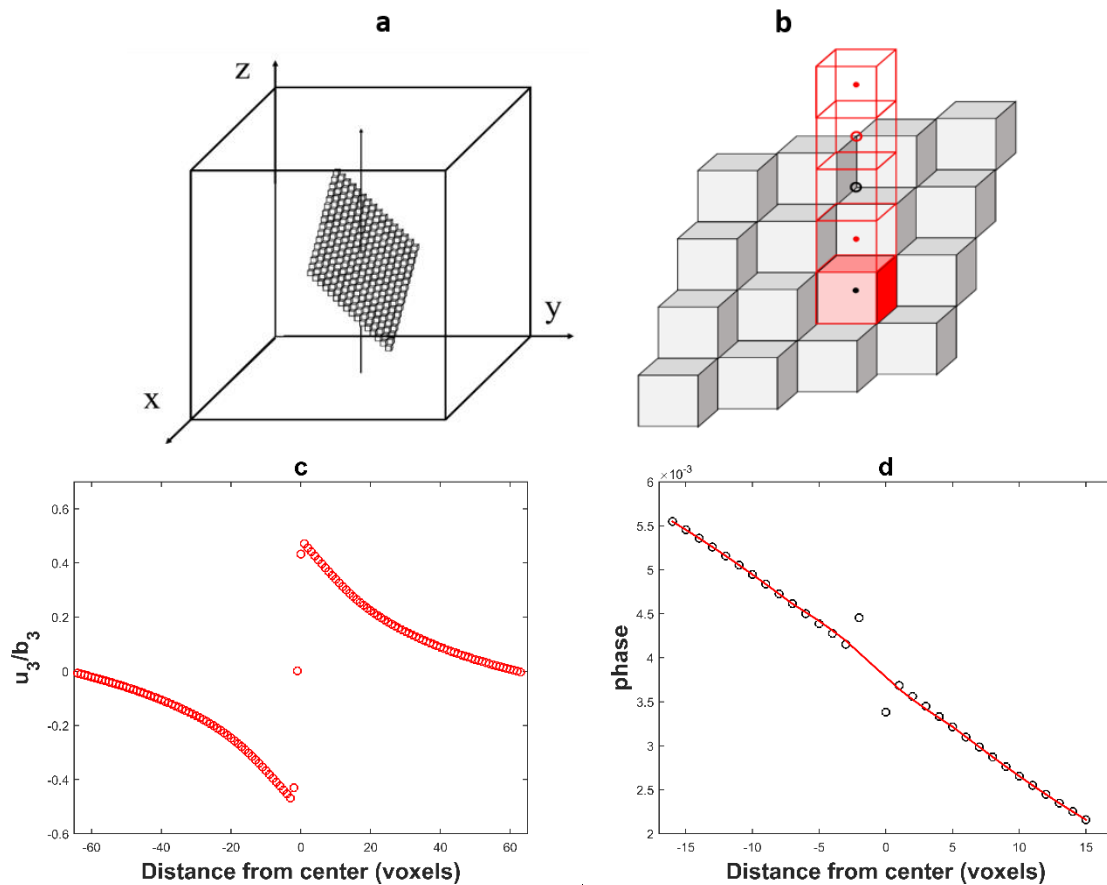
$$\varepsilon_{ij}^* = \frac{A_s}{2V} (n_i b_j + n_j b_i) \quad (6)$$

161 where  $A_s$  is the area on which planes with normal  $\mathbf{n}(n_1, n_2, n_3)$  has slipped by a relative amount  
 162  $\mathbf{b}(b_1, b_2, b_3)$  and  $V$  is the volume occupied by the loop [40,41]. As before, the dislocation loop is 32  
 163 voxels wide in the  $x$  and  $y$  directions, and 1 voxel thick but now with a  $z$  position such that  $x + y +$   
 164  $z = \text{constant}$ . The displacement has been computed at the center of voxels with the periodized  
 165 operator  $\mathbf{B}'$  along  $z$  (figure 2b). As in figure 1c, the displacement in the center of a voxel belonging  
 166 to the loop plane (black dot in the reddish transformed voxel in figure 2b) is zero. The displacement  
 167 in the first neighboring voxels (red dot in figure 2b) are shifted relative to the expected position, so  
 168 that the displacement difference between these voxels is significantly lower than  $\mathbf{b}$ , see figure 2c. It  
 169 can be checked in figure 2b that each of these voxels shares three faces with a transformed voxel. A  
 170 more detailed analysis shows that the second neighbors (which share three edges with transformed  
 171 voxels) are also slightly shifted in the opposite direction. The result is shown in figure 2d with:  
 172 a strong localized oscillation of the phase (taken here as the displacement modulo  $\mathbf{b}$ ).

173 Although the amplitude of this shift is small (less than 10% of the Burgers vector) it has  
 174 unwanted consequences on the diffraction peak simulation:

- 175 • The dislocation loops are surrounded by four impaired layers of voxels: As the scattered X-Ray  
 176 amplitude is proportional to the Fourier transform of  $\mathbf{G} \cdot \mathbf{u}$  (see equation (8) in section 4) we can  
 177 expect a phantom streak in the intensity in a direction perpendicular to the loop plane.
- 178 • The displacement field near the edges of the loop (near the dislocation line) will be quite different  
 179 from its expected value, and the strain field will not vary with the distance  $r$  to the dislocation  
 180 line as  $1/r$ . This will strongly affect the tails of the diffraction peaks

181



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**Figure 2.** (a) Modeling of a squared dislocation loop in a (111) plane as a layer of voxels with eigenstrain; (b) position of the computed points relative to the transformed voxels with eigenstrains; (c) Plot of the displacement field  $u_3$  (normalized by  $b_3$ ) along the  $z$  direction for dislocation loop

186 illustrated on figure 2. (d) Local oscillation of the phase due to the voxelization of the dislocation loop  
 187 (the representation is made for 32 voxels centered in the unit cell along z direction). The red line is  
 188 approximately equal to the phase expected for this displacement field.

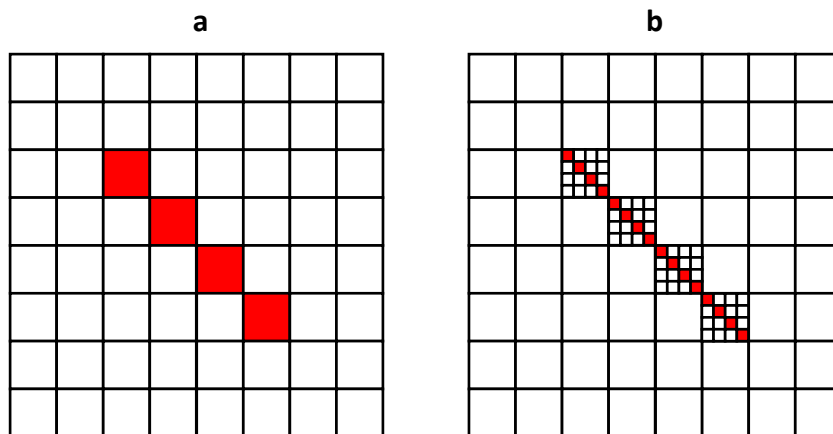
### 189 3. Sub-voxelization method to correct voxelization effects.

#### 190 3.1. Sub-voxelization method

191 The (conceptually) simplest way to remove this voxelization artifact would be to work on a  
 192 multiple grid (to multiply the number of voxels along each direction by 2, 4, or more), then to  
 193 downsample the displacement field data. In that case, FFT algorithms would lose much of their  
 194 interest due to these more demanding computational efforts. We show below that this can be done  
 195 in a more economical way by applying a patch to the FFT-computed displacement field. The basic  
 196 method is to compute *on the same grid* the difference vector:

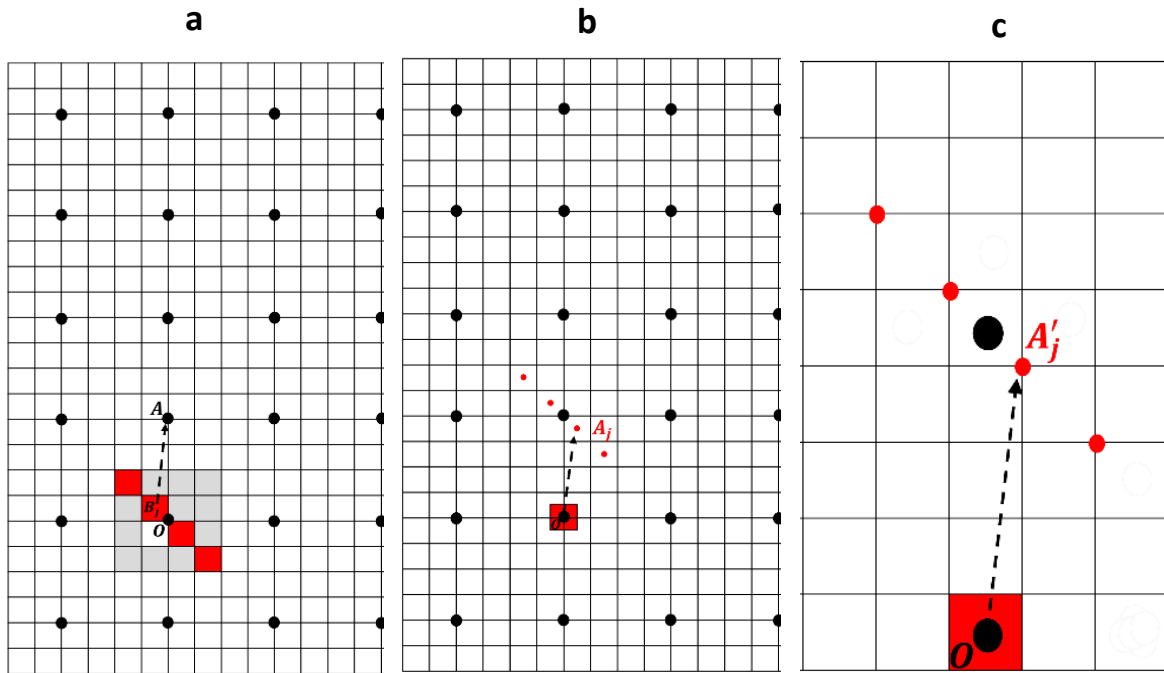
$$197 \Delta_i(\mathbf{x}) = u_i^{sub}(\mathbf{x}) - u_i^{hom}(\mathbf{x}) \quad (7)$$

198 where  $u_i^{sub}(\mathbf{x})$  is the displacement vector calculated for voxels where this eigenstrain is  
 199 concentrated on a single plane of sub voxels (figure 3b) and  $u_i^{hom}$  the displacement field in direction  
 200 i of voxels with a uniform eigenstrain (figure 3a). For the sake of clarity, we use 2D diagrams in Figure  
 201 3, but here the technique is applied to real 3D problems.



202 **Figure 3.** 2D representation of a dislocation loop in a tilted plane on a  $(8 \times 8)$  FFT grid. (a) With a  
 203 homogeneous eigenstrain in the voxels occupied by the dislocation loop. (b) With each voxel  
 204 subdivided into  $4 \times 4$  sub-voxels, only 4 of which are eigenstrained.

205 In order to compute the displacement due to sub-voxels, we use a  $N \times N$  ( $N \times N \times N$ ) grid for  
 206 2D (resp. 3D) problems where each voxel can be subdivided into  $n \times n$  ( $n \times n \times n$ ) sub voxels. Only  
 207  $n \times n$  sub voxels are submitted to an eigenstrain field. At a point  $\mathbf{A}$  of the grid (black dots, figure  
 208 4a), we need to compute the sum of the displacements  $\mathbf{u}_i^j$  due to the  $n$  ( $n \times n$ ) sub voxels  $j$  (center  
 209  $\mathbf{B}_j$ ) within a voxel centered at point  $\mathbf{O}$ . This sum is equivalent to the sum of the displacements due  
 210 to a strained sub voxel at point  $\mathbf{O}$  on the grid points  $\mathbf{A}_j$  such as  $\mathbf{OA}_j = \mathbf{B}_j\mathbf{A}$  (figure 4b). It is also  
 211 equivalent to the sum of the displacements  $\mathbf{u}_i^j$  due to a *full* voxel at point  $\mathbf{O}$  on the initial grid on  
 212 points  $\mathbf{A}'_j$  such as  $\mathbf{OA}'_j = n\mathbf{B}_j\mathbf{A}$  (figure 4c). The only difference between these last two sums is due to  
 213 the long-range strain field, and approximately results in a linear drift of the displacement. As the end  
 214 of the vectors  $\mathbf{OA}'_j$  does not lie on the grid points (voxel centers) but on the corners of the voxels, the  
 215  $\mathbf{u}_i^j$  displacements must be calculated with the shifted operator  $\mathbf{B}''$  (equation (5)). A last point is the  
 216 scaling of the  $\mathbf{u}_i^j$  and  $\mathbf{u}_i^j$  sums during the operations of figure 4. To keep the one Burgers vector  
 217 jump between both sides of the sub voxels plane in Figure 4a, the eigenstrain in the sub voxels must  
 218 be multiplied by  $n$ . The backwards change of scale requires a division by  $n$ : there is no scaling factor  
 219 between  $u_i^{hom}$  and  $u_i^{sub} = \sum u_i^j$ .



220

221 **Figure 4.** (a). 2D representation of the computational grid. Black dots correspond to the voxels center.  
 222 A voxel with center  $O$  is discretized in  $4 \times 4$  in 2D ( $4 \times 4 \times 4$  in 3D) sub-voxels. Some sub-voxels  
 223 contain an eigenstrain (red sub-voxels). We want to compute the displacement field at voxel centered  
 224 at point  $A$ , due to these deformed sub-voxels centered at  $B_j$ . (b) Effect of one deformed sub-voxel  
 225 centered at  $O$  on a row of sub-voxels centered at  $B_j$  such as  $OA_j = B_j A$ . The sum of these effects is  
 226 equal to the previous displacement field. (c) Effect of deformed voxels centered at  $O$  on a row of voxels  
 227 (computed at corners  $A'_j$  using Green operator  $B''$ ) such as  $OA'_j = n B_j A$ . This sum is equal to  
 228 previous wanted sum.

229 We need to compute  $\Delta_{ij\_pl}(\mathbf{x})$  the difference in displacement in direction  $i$  due to a voxel which  
 230 belongs to the plane "pl" (for fcc "pl" is equal to  $(111), (\bar{1}\bar{1}\bar{1}), (1\bar{1}\bar{1}), (11\bar{1})$ ) of a dislocation loop  
 231 with a Burgers vector  $j$  at a position  $\mathbf{x}$  relative to the transformed voxel. In practice, in a material with  
 232 cubic symmetry, it is sufficient to compute  $\Delta_{13\_ (111)}(\mathbf{x})$  and  $\Delta_{33\_ (111)}(\mathbf{x})$ , and to use the symmetries  
 233 of the cube (fourfold  $[001]$  axis, threefold  $[111]$  axis, and  $(1\bar{1}0)$  symmetry plane) (and suitable  
 234 exchanges of the components of  $\mathbf{x}$ ) to obtain the required components. As it can be seen in figure 2b,  
 235  $\Delta_{ij\_pl}(\mathbf{x})$  is non-zero only for the neighbors of the transformed voxel, except the drift due to the long  
 236 range strain alluded above. The final recipe to compute  $\Delta_{ij\_pl}(\mathbf{x})$  and use the patch becomes:

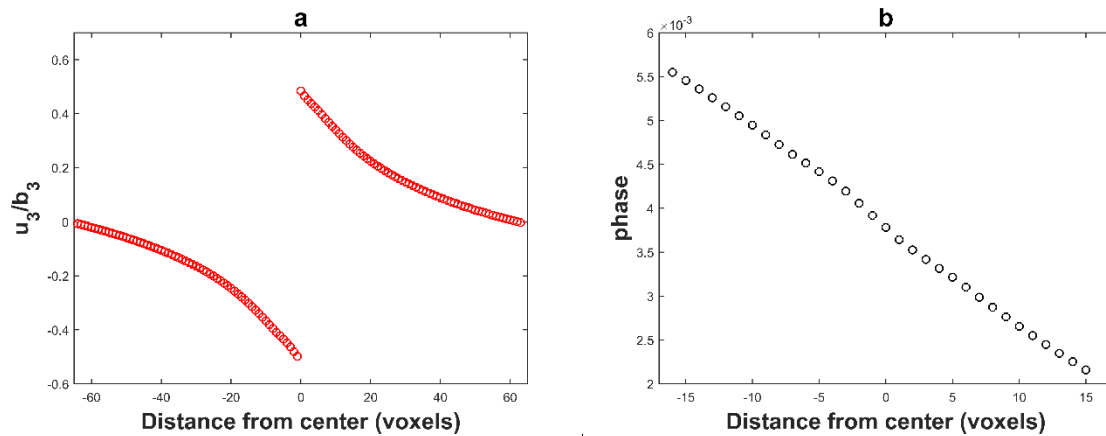
- 237 • Compute the field  $\mathbf{c}^0: \boldsymbol{\varepsilon}^*$  defined in equation (1) for an isolated voxel with the eigenstrain  
 238 associated to a dislocation loop (equation (6)) with a Burgers vector  $[001]$  in a  $(111)$  plane (see  
 239 figure 2).
- 240 • Compute the displacement field in directions  $x(\mathbf{u}_1^{hom})$  and  $z(\mathbf{u}_3^{hom})$  at the voxels' center around  
 241 the transformed voxel by convolution with the discrete periodized operator  $\mathbf{B}'$  (equation (4))
- 242 • Compute the displacement field in directions  $x$  and  $z$  at the voxels' corners around the  
 243 transformed voxel by convolution with the shifted operator  $\mathbf{B}''$  (equation (5))
- 244 • Calculate the  $\mathbf{u}_1^{sub} = \sum \mathbf{u}_1^j$  and  $\mathbf{u}_3^{sub} = \sum \mathbf{u}_3^j$  sums ( $n \times n$  terms for each sum) as in figure 4c,  
 245 then the raw  $\Delta_{13\_ (111)}(\mathbf{x})$  and  $\Delta_{33\_ (111)}(\mathbf{x})$  for  $(x_1, x_2, x_3)$  going from  $-3$  to  $3$  times the voxel size  
 246  $t$ .
- 247 • Use the farthest voxels to correct the drift of the components so that all terms for large  $\mathbf{x}$  are  
 248 zero, and keep only the terms for the first three neighbors non zero. .

249 The patch can then be applied on the raw (FFT-based) displacement field by adding the  
 250 convolution of all transformed voxels of the different slip systems by the relevant  $\Delta_{ij\_pl}(\mathbf{x})$ .



## 251 3.2. Results

252 For tests, we used the same  $128 \times 128 \times 128$  grid as above, and the transformed voxel was  
 253 divided into  $8 \times 8 \times 8$  sub voxels (using a reference medium with the same elastic constants as before).  
 254 Only the final values in units of  $b$  (after drift correction) of  $\Delta_{13,(111)}(\mathbf{x})$  and  $\Delta_{33,(111)}(\mathbf{x})$  are used  
 255 and others components are obtain by symmetries (Appendix A).



256 **Figure 5.** (a) Plot of the displacement field  $u_3$  (normalized by  $b_3$ ) along the  $z$  direction for dislocation  
 257 loop illustrated on figure2. Artifacts are removed by sub-voxel method described above. (b) the phase  
 258 (i.e. the displacement modulo a Burgers vector). With this correction, the phase is almost continuous.  
 259

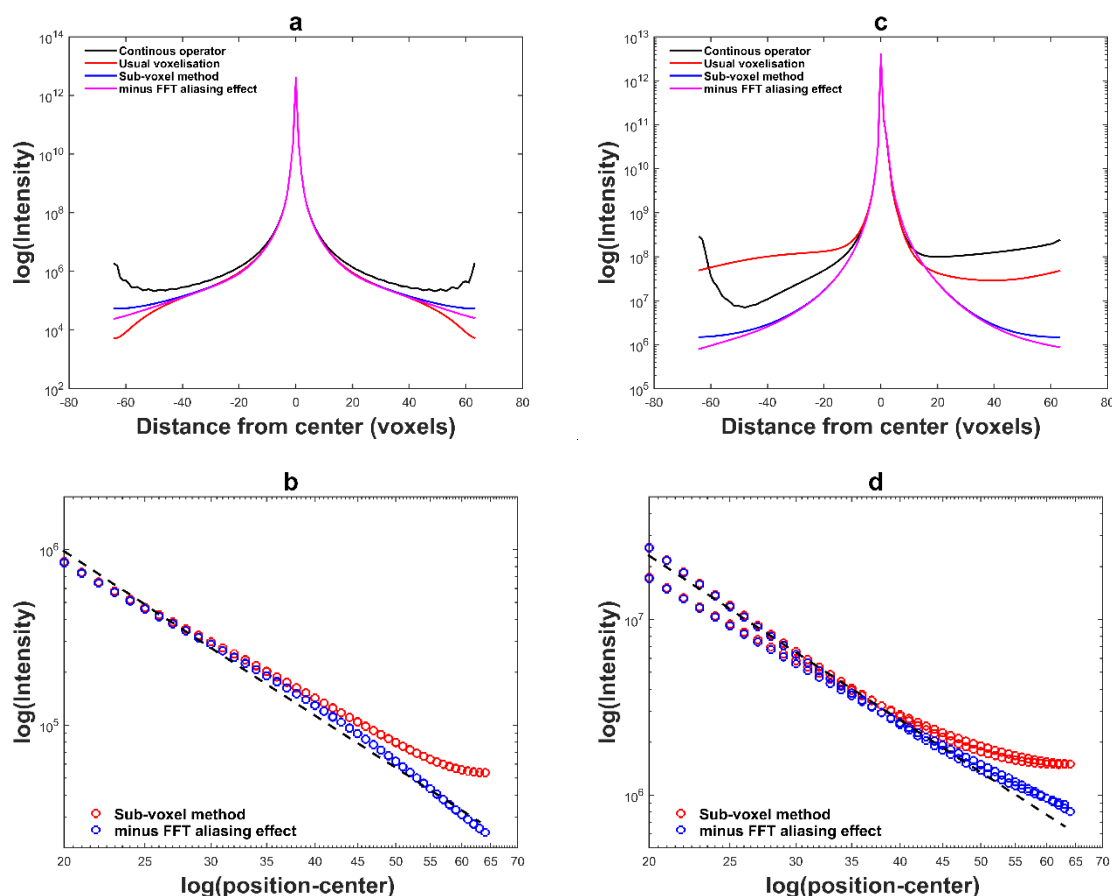
260 The patch was used on the same configuration as in figure2. Figure 5a shows the resulting  
 261 displacement field and figure 5b the phase (i.e. the displacement modulo a Burgers vector) in Burgers  
 262 vector units. As it can be observed from figure 5a, the artifacts of the displacement field have  
 263 disappeared. In addition, the resulting phase varies smoothly even during the crossing of the  
 264 dislocation loop, see figure 5b.

## 265 4. Application on diffraction peak simulation

266 In this section, we show simulated diffraction peaks in order to point the effects of voxelization  
 267 artifacts and of the patch on numerical results. Under kinematical conditions and assuming a  
 268 coherent beam, the amplitude of a diffracted wave at a position  $\mathbf{q}$  in the vicinity of a reciprocal  $\mathbf{G}$   
 269 lattice vector is [14,18,42–44]:

$$270 \quad A(\mathbf{q}) = FT[A_0(\mathbf{r}) \times F(\mathbf{G}, \mathbf{x}) \times \exp(-2i\pi \mathbf{G} \cdot \mathbf{u}(\mathbf{x}))] \quad (8)$$

271 where  $\mathbf{x}$  is the position of the scattering atom,  $A_0(\mathbf{x})$  is the amplitude of the incidence wave,  $F(\mathbf{G}, \mathbf{x})$   
 272 is the local structure factor and  $\mathbf{u}(\mathbf{x})$  the displacement field. The scattered intensity is  $I(\mathbf{q}) = |A(\mathbf{q})|^2$ .  
 273 For a face-centered cubic crystal, this intensity is non zero when  $\mathbf{G} (h, k, l)$  is such as  $h, k,$  and  $l$  have  
 274 the same parity. Here two diffraction vectors  $\mathbf{G} (200)$  and  $\mathbf{G} (002)$  are used. They respectively  
 275 correspond to  $\mathbf{G} \cdot \mathbf{b} = 0$  and  $\mathbf{G} \cdot \mathbf{b} = 1$ . The 3D diffracted intensity has been calculated using the FFT  
 276 instead of the continuous Fourier Transform, then summed in the planes perpendicular to the  $\mathbf{G}$   
 277 vector to obtain a linear plot along  $\mathbf{G}$  equivalent to a  $I(2\theta)$  plot. In figures 6a ( $\mathbf{G} (200)$ ) and 6c ( $\mathbf{G}(002)$ ),  
 278 we show the diffracted intensity (logarithmic scale) as a function of the pixel position  $i$ , and in figures  
 279 6b and 6d a logarithmic/logarithmic plot of the intensity vs.  $|i - i_0|$  where  $i_0$  is the center of the  
 280 peak. In order to only study the effect of the displacement fields, we set  $A_0(\mathbf{x}) = 1$  and  $F(\mathbf{G}, \mathbf{x}) = 1$   
 281 for these simulations.



282

283

284 **Figure 6.** Simulated diffracted intensity as a function of the pixel position (logarithmic scale). 3D  
 285 configuration is represented in 1D plot by making sum in each plane along an x-axis. Different way  
 286 for computing the displacement fields are studied for a dislocation loop with a  $[0\bar{1}1]$  Burgers vector  
 287 lying in a (111) slip plane. (a) Diffracted vector studied is  $\mathbf{G}$  (200) corresponding to  $\mathbf{G}\cdot\mathbf{b} = 0$ . (b)  
 288 log/log representation of the intensity vs.  $|i - i_0|$ . (c) and (d) Same as (a) et (b) but the studied  
 289 diffracted vector is  $\mathbf{G}$  (002).

290 The peak shape near the top of the peaks is the same for both computing methods. It is perfectly  
 291 symmetric in the  $\mathbf{G}\cdot\mathbf{b} = 0$  case and exhibits a bump on the right side for  $\mathbf{G}\cdot\mathbf{b} = 1$ . Their long-range  
 292 behavior is however quite different. When the displacement field has been calculated with the usual  
 293 truncated operator (black line), a phantom peak is observed at large  $|i - i_0|$  (at large  $q$ ), which is due  
 294 to the short period oscillations near the displacement field discontinuity (Figure 1a). The behavior of  
 295 the peak calculated with the modified Green operator (blue curve) is only slightly better: the intensity  
 296 at large  $q$  is underestimated in one case and overestimated in the other. When the intensity has been  
 297 calculated with the sub voxel patch (red curve) the long range intensity follows the expected  
 298  $I_0|i - i_0|^{-3}$  law [45,46]: the peak tails are indeed related to the highly distorted zones near the  
 299 dislocations' cores. However, the red curve saturates at very large  $q$ . We suppose this is due to the  
 300 use of the Fast Fourier Transform instead of the continuous Fourier Transform in the calculation of  
 301 the scattered amplitude (equation (8)): The plot of figure 6 represents only one period in Fourier  
 302 space, and is repeated over and over on all Fourier space. We can now calculate the intensity of the  
 303 tails of these repetitions:

$$304 \quad I_{neib.} = \sum I_0|i - i_0 - 128m|^{-3} \quad (9)$$

305 where  $m$  varies from -5 to 5 (zero excluded). We obtain the pink curve at the bottom of figures 5a and  
 306 5c. If we now plot the difference between the red intensity curve and this pink background line, we  
 307 obtain the green curve. On the log./log. plots, figure 6b and 6d it can be checked that this curve follows  
 308 the  $I_0|i - i_0|^{-3}$  law to the end. Thus, the residual error in the intensity computed by FFT results of  
 309 the FFT itself, and not from a residual error on the sub voxel corrected displacement field. If the

310 number of voxels is increased to  $512^3$  or  $1024^3$  while keeping the physical size of the Representative  
311 Volume constant this residual error should fall down to undetectable levels.

## 312 5. Conclusions

313 In this paper, we showed that although the use of a periodized Green operator in the FFT-based  
314 method improves the final displacement field solution in a Representative Volume containing  
315 discontinuities (dislocation loops), artifacts due to the voxelization of the dislocation loop planes are  
316 still present with respect to analytical solutions. These artifacts have unwanted consequences on the  
317 tails of diffraction peaks simulated by using this displacement field as input data.

318 We have introduced a patch which corrects these artifacts by simulating the displacement field  
319 which would be obtained with a much finer voxelization without need to do the computations on a  
320 finer grid. A simple construction method for this patch has been given and the patch can be used in  
321 a single post-processing step to modify the initial FFT-based displacement field.

322 The modified displacement field has been used to simulate one-dimensional diffraction peaks.  
323 The procedure strongly improves the shape of the peaks' tails, i.e. it gives a good description of the  
324 displacement field near the dislocation lines.

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331 Ribarik helped in constructing the computer code and helped in analyzing results; Stéphane Berbenni  
332 helped in developing the first theoretical part of the paper. The paper was written by Komlavi S. Elo,  
333 Alain Jacques and Stéphane Berbenni.

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## 335 Appendix A

336  $\Delta_{33_{(111)}}(x_1, x_2, x_3)$  and  $\Delta_{13_{(111)}}(x_1, x_2, x_3)$  have these symmetries due to the permutation  
337 properties of the plan **(111)**

$$338 \Delta_{33_{(111)}}(x_1, x_2, x_3) = \Delta_{33_{(111)}}(x_2, x_1, x_3)$$

$$339 \Delta_{33_{(111)}}(x_1, x_2, x_3) = -\Delta_{33_{(111)}}(-x_1, -x_2, -x_3)$$

$$340 \Delta_{13_{(111)}}(x_1, x_2, x_3) = -\Delta_{13_{(111)}}(-x_1, -x_2, -x_3)$$

341 The others values of  $\Delta_{ij_{(111)}}(\mathbf{x})$  are given as function of  $\Delta_{33_{(111)}}(x_1, x_2, x_3)$  and  $\Delta_{13_{(111)}}(x_1, x_2, x_3)$ :

$$342 \Delta_{11_{(111)}}(x_1, x_2, x_3) = \Delta_{33_{(111)}}(x_3, x_2, x_1) \quad \Delta_{12_{(111)}}(x_1, x_2, x_3) = \Delta_{13_{(111)}}(x_1, x_3, x_3)$$

$$343 \Delta_{22_{(111)}}(x_1, x_2, x_3) = \Delta_{33_{(111)}}(x_1, x_3, x_2) \quad \Delta_{31_{(111)}}(x_1, x_2, x_3) = \Delta_{13_{(111)}}(x_3, x_2, x_1)$$

$$344 \Delta_{32_{(111)}}(x_1, x_2, x_3) = \Delta_{13_{(111)}}(x_3, x_1, x_2) \quad \Delta_{21_{(111)}}(x_1, x_2, x_3) = \Delta_{13_{(111)}}(x_1, x_3, x_2)$$

$$345 \Delta_{23_{(111)}}(x_1, x_2, x_3) = \Delta_{13_{(111)}}(x_2, x_1, x_3)$$

346 The value of  $\Delta_{33}(x_1, x_2, x_3)$  and  $\Delta_{13}(x_1, x_2, x_3)$  for the remaining plane  $(\bar{1}11), (1\bar{1}1), (11\bar{1})$  are  
347 obtained using these symmetries:

$$348 \Delta_{33_{(\bar{1}11)}}(x_1, x_2, x_3) = \Delta_{33_{(111)}}(x_2, -x_1, x_3) \quad \Delta_{13_{(\bar{1}11)}}(x_1, x_2, x_3) = \Delta_{13_{(111)}}(-x_1, x_2, x_3)$$

$$349 \Delta_{33_{(1\bar{1}1)}}(x_1, x_2, x_3) = \Delta_{33_{(111)}}(-x_2, x_1, x_3) \quad \Delta_{13_{(1\bar{1}1)}}(x_1, x_2, x_3) = \Delta_{13_{(111)}}(x_1, -x_2, x_3)$$

$$350 \Delta_{33_{(11\bar{1})}}(x_1, x_2, x_3) = -\Delta_{33_{(111)}}(x_2, x_1, -x_3) \quad \Delta_{13_{(11\bar{1})}}(x_1, x_2, x_3) = -\Delta_{13_{(111)}}(x_1, x_2, -x_3)$$

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