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Electric field gradients in simple tetragonal lattice at interstitial site

D P VERMA*, B KUMAR and H C VERMA

Department of Physics, *Department of Mathematics, Patna Science College, Patna University, Patna 800005, India

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Abstract. Electric field gradient (EFG) is calculated at the centre of the cell in the simple tetragonal crystal. The method uses Euler-Maclaurin summation formula and makes the planewise summation in the direct crystal space without any special regrouping of charges in point charge model. The results are in fair agreement with previous results of de Wette on the same system using Fourier transform to reciprocal space.

Keywords. Electric field gradients; lattice sum; convergence; simple tetragonal crystal, Euler-Maclaurin formula; double series.

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1. Introduction

In a previous communication (Verma *et al* 1983) a new method to calculate the lattice contribution to electric field gradients (EFG) at a nuclear site in simple tetragonal crystal was developed. The method uses Euler-Maclaurin (EM) summation formula to evaluate the infinite series and the error terms are estimated by using the same formula for a related finite sum. The sum is evaluated in the direct crystal space unlike most of the previous methods using Fourier transform to reciprocal space. Also no special regrouping of charges is required. The same method has been used here to calculate the EFG at the centre of the cell (1/2, 1/2, 1/2) in simple tetragonal crystal. These results together with those of the above referred paper immediately give EFG in tetragonal close-packed (TCP) crystals.

2. Notations

The following notations will be used

n_1, n_2, n_3 stand for integers.

$x^* = x + 1/2$, $P = n_3^{*2} c^2/a^2$, $Q = P + 1/4$,

$A(n) = P + n^{*2}$ and $B(n) = A(n) + 1/4$.

3. Details of calculation

The lattice sum of electric field gradient due to the positive ions of the crystal is

$$\mathrm{eq}_{\mathrm{latt}} = \sum_i \frac{Ze}{4\pi\varepsilon_0} \frac{3z_i^2 - r_i^2}{r_i^5}, \tag{1}$$

where z_i is the z-coordinate and r the distance of the charge Ze with respect to the site at which EFG is being calculated.

Taking the centre of a unit cell as origin, the coordinates of various lattice points are given by $(n_1^* a, n_2^* a, n_3^* c)$, where n_1, n_2, n_3 run through integrers. The contribution to summation (1) from this point is

$$\frac{Ze}{4\pi\varepsilon_0 a^3} F(n_1, n_2, n_3).$$

where

$$F(n_1, n_2, n_3) = \frac{2P - n_1^{*2} - n_2^{*2}}{(P + n_1^{*2} + n_2^{*2})^{5/2}}.$$

Thus the lattice sum in units of $Ze/(4\pi\varepsilon_0 a^3)$ is

$$S_{1/2,\,1/2,\,1/2} = \sum_{n_1, n_2, n_3 = -\infty}^{\infty} F(n_1, n_2, n_3)$$

$$= 8 \sum_{n_1, n_2, n_3 = 0}^{\infty} F(n_1, n_2, n_3). \tag{2}$$

As discussed in Verma *et al* (1983), we shall employ planewise summation *i.e.* we shall evaluate the EFG at the origin from planes perpendicular to the c-axis and then add the EFG from different planes. As we go away from the origin the effect of discreteness of ion positions in a plane will become smaller and smaller, the plane will behave more as a uniformly charged plane sheet and EFG will become very nearly zero. We therefore expect that only a small number of planes will be effective. The calculations show that two or three planes above the origin and the same number below it are sufficient for convergence.

3.1 *Contribution of plane* $z = n_3^* c$

The contribution of plane $z = n_3^* c$ to this triple sum is

$$U(n_3) = \sum_{n_1, n_2 = 0}^{\infty} F(n_1, n_2, n_3). \tag{3}$$

The EM formula (Hildebrand 1956) is

$$\sum_{n=M}^{N} f(n) = \int_M^N f(x)\,\mathrm{d}x + \tfrac{1}{2}\{f(N) + f(M)\} + \int_M^N P_1(x) \frac{\mathrm{d}f(x)}{\mathrm{d}x}\,\mathrm{d}x \tag{4}$$

where $P_1(x) = x - \frac{1}{2}$ for $0 \leqslant x < 1$ and is defined outside this region by $P_1(x+1)$

$= P_1(x)$. Using this formula to (3) we get,

$$U(n_3) = \sum_{n_1=0}^{\infty} \frac{2P}{A^2(n_1)} - \sum_{n_1=0}^{\infty} \frac{1}{A(n_1)} + \sum_{n_1=0}^{\infty} \left[\frac{1}{2B^{1/2}(n_1)} \left(\frac{1-4P}{A(n_1)} - \frac{2P}{A^2(n_1)} - \frac{1-4P}{B(n_1)} + \frac{3P}{B^2(n_1)} \right) \right] + \sum_{n_1=0}^{\infty} \int_0^{\infty} P_1(x) \frac{dF(x)}{dx} dx, \tag{5}$$

where $F(x) = F(n_1, x, n_3)$.

The first two series can be summed exactly, using Cauchy's residue formula (Spiegel 1964), giving a combined value $-\frac{1}{2}\pi^2 \operatorname{sech}^2 \pi\sqrt{P}$ and the next four series can be expanded using EM formula (4). This gives

$$\begin{aligned} U(n_3) &= -\tfrac{1}{2}\pi^2 \operatorname{sech}^2 \pi\sqrt{P} + \left(\frac{6P+5/2}{16P^{*3/2}Q^2} - \frac{3}{8P^{*5/2}} - \frac{1}{4Q^2} \right) + \varepsilon(\infty) \\ &= -\tfrac{1}{2}\pi^2 \operatorname{sech}^2 \pi\sqrt{P} + H(n_3) + \varepsilon(\infty), \end{aligned} \tag{6}$$

where $\varepsilon(\infty)$ contains all the integrals involving $P_1(x)$.

To estimate $\varepsilon(\infty)$ we apply the above procedure to the finite sum

$$U_N(n_3) = \sum_{n_1, n_2 = 0}^{N} F(n_1, n_2, n_3)$$

and get

$$U_N(n_3) = H(n_3) + \frac{1}{4Q^2} + H(N, n_3) + g(N, n_3) + \varepsilon(N), \tag{7}$$

where $\varepsilon(N)$ contains all integrals involving $P_1(x)$,

$$H(N, n_3) = \frac{1}{B^{1/2}(N)} \left(\frac{N^{*2} - \frac{1}{2}(N+1)}{A(N)} + \frac{N^{*2}}{2A^2(N)} + \frac{N^*(2P-1)}{4Q^2} \right) - \frac{1}{B^{3/2}(N)} \left(N(N+1) + \frac{N^{*3}P}{2Q^2} \right) - \frac{3(N^{*2} + 1/4)}{4B^{5/2}(N)},$$

while

$$g(N, n_3) = \sum_{n=0}^{N} \frac{3PN^*}{A^2(n)(A(n) + N^{*2})^{1/2}} - \sum_{n=0}^{N} \frac{PN^{*3}}{A^2(n)(A(n) + N^{*2})^{3/2}} - \sum_{n=0}^{N} \frac{N^*}{A(n)(A(n) + N^{*2})^{1/2}} + \sum_{n=0}^{N} \frac{2P - n^{*2} - N^{*2}}{2(A(n) + N^{*2})^{5/2}}.$$

Hence by (7),

$$\varepsilon(N) = \sum_{n_1, n_2 = 0}^{N} F(n_1, n_2, n_3) - g(N, n_3) - H(N, n_3) - H(n_3) - \frac{1}{4Q^2}$$

and by (6),

$$U(n_3) = -\tfrac{1}{2}\pi^2 \operatorname{sech}^2 \pi\sqrt{P} + \sum_{n_1, n_2 = 0}^{N} F(n_1, n_2, n_3) - g(N, n_3)$$

$$- H(N, n_3) - \frac{1}{4Q^2} + \varepsilon(\infty) - \varepsilon(N). \tag{8}$$

It was shown in Verma *et al* (1983) that if $P_1(x)$ terms are obtained with $N = 80$ and substituted for the corresponding error terms with $N = \infty$, the uncertainty is less than 10^{-6}. The present expression of $P_1(x)$ terms are similar and hence we take $N = 80$ and neglect $|\varepsilon(\infty) - \varepsilon(N)|$ for numerical calculations.

Thus we get contribution to EFG at the centre of cell from the plane $z = n_3^* c$.

Contributions from different planes $n_3 = 0, 1, 2, 3, \ldots$ were numerically evaluated using (8). It was found that only five or six planes, two or three planes above and two or three below were sufficient for convergence in z-direction.

To minimise the truncation error, special care was taken while programming and the terms of too different magnitudes, were not added directly.

4. Results and discussion

The results for different c/a are listed in table 1 together with the available calculation of de Wette (1961) using Fourier transforms. The good agreement between the sets shows that the EM formula may be effectively used to improve the slow convergence of lattice sums.

A TCP crystal can be imagined to be a combination of two simple tetragonal crystals having same lattice parameters displaced with respect to one another by $(a/2, a/2, c/2)$. The regular site for one subcrystal is the centre of a cell of other subcrystal. The EFG at a regular site in TCP crystal can therefore be obtained by adding the EFG's at a regular site and at the centre of cell *i.e.* by adding the corresponding results of Verma *et al* (1983) and that of table 1.

Table 1. Lattice EFG at the centre of cell in simple tetragonal crystal in units of $Ze/(4\pi\varepsilon_0 a^3)$.

c/a	Present values	Values from de Wette (1961)
1·00	−8·37757	−8·378
1·10	−6·55387	−6·554
1·30	−3·89969	−3·8997
1·50	−2·25279	−2·25279
1·80	−0·95201	−0·9520161
2·00	−0·52689	−0·5269000
2·25	−0·24829	−0·2482920
2·50	−0·11584	−0·1158417

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