Temperature variation of electric field gradient in scandium metal

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Abstract. Electric field gradient (EFG) in scandium metal has been evaluated at temperatures 11 K and 293 K using band wave functions determined in the temperature dependent model potentials. The results of net EFG obtained are $-3.756 \times 10^{13}\,\text{esu/cm}^3$ and $-8.009 \times 10^{13}\,\text{esu/cm}^3$ at 11 K and 293 K respectively. The agreement with available experimental result is reasonably good.

Keywords. Electric field gradient; temperature variation; scandium metal; model potential.

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1. Introduction

Electric field gradient in a solid arises if its charge distribution has lower symmetry than cubic. In non-cubic metals both the localised ions and the itinerant conduction electrons contribute to EFG. The contribution from the localised ions, referred to as the lattice contribution [1], when evaluated in point-ion approximation [2], is expressed as a simple function of lattice parameters. This is particularly true in the hexagonal-close-packed (hcp) solids. The contribution from the conduction electrons, on the other hand, requires a more involved and complex procedure for its evaluation. The standard procedure often used for this purpose is the energy band calculation which provides wave functions for all the occupied electron states. Using these wave functions, EFG is evaluated.

Changes in the temperature bring about changes in both lattice and electron-contribution to EFG. In the point-ion model [1] the effect of temperature variation on the lattice EFG can be included through the change in the lattice parameters. But for electronic contribution, the use of changed lattice parameters is not enough. This is because the potential that determines the electron distribution also changes with temperature. This will not only cause changes in the radial character of the wave function but may also bring about a change in the distribution of electrons in Fermi volume. As a consequence of the latter, electron states which are occupied/(unoccupied) at one temperature may become unoccupied/(occupied) at a different temperature and this may change the contribution to EFG.

One way of getting the changed electron-distribution in Fermi volume due to variation in temperature is by carrying out the energy band calculations with tempera-ture-dependent potential. The latter has been worked out by Kasowski [3]. By treating electron-phonon interaction, he [3] has shown that the Fourier integrals of pseudo-potential at two different temperatures are related by some simple relation involving

Debye–Waller factor [3]. Thus, using this formalism it is possible to obtain the Fourier integral of pseudo-potential at any temperature from those available at a known temperature. Once these are determined, they can be used in the energy band calculations to obtain energy and wave functions of occupied electron states at any desired temperature. This procedure has been used in the past for the study of temperature-dependence of Knight-shift [3] and spin susceptibility [4] in metals.

In the present work we have followed the above procedure for evaluating the EFG of the conduction electrons at two temperatures, namely, 11 K and 293 K. Although the procedure is general enough to be applicable for other temperatures, the present work is limited to the above two temperatures because lattice parameters for Sc are currently available [5, 6] only at these two temperatures.

The paper is organized as follows. In § 2 we briefly describe the theory of temperature dependence of EFG. Results and discussion are presented in § 3. Section 4 summarizes the conclusions.

2. Theory

Energy band calculations using non-local model potential are very common. The details of this procedure applied to scandium metal at 293 K are described elsewhere [7, 8]. Here we will briefly go over the necessary theory for the sake of completeness. In atomic units ($e^2 = 2$, $\hbar = 1$, $m = \frac{1}{2}$) the Hamiltonian of an electron in a periodic solid is given by

$$H = -\nabla^2 + V_m, \tag{1}$$

where V_m is a suitable model potential which, in general, has a local and non-local part. The bare-ion model potential whose parameters are tabulated [9] is screened by the same dielectric function as used in the previous work [7].

The model wave function χ_t, where t denotes the band index, is expanded on the basis of plane waves,

$$|\chi_t(\mathbf{k})\rangle = \sum_{\mathbf{K}} C_t(\mathbf{k}, \mathbf{K})|\mathrm{PW}(\mathbf{k} + \mathbf{K})\rangle, \tag{2}$$

where the coefficients $C_t(\mathbf{k}, \mathbf{K})$ and the band energy $E_t(\mathbf{k})$ are obtained as solutions of the secular equation,

$$|H_{\mathbf{k}+\mathbf{K}, \mathbf{k}+\mathbf{K}'} - E_t(\mathbf{k})\delta_{\mathbf{K},\mathbf{K}'}| = 0. \tag{3}$$

Once the coefficients $C_t(\mathbf{k}, \mathbf{K})$ are determined, the true wave function $|\Psi_t(\mathbf{k})\rangle$ is constructed from the model wave function $|\chi_t(\mathbf{k})\rangle$ by orthogonalizing the latter to the core states in the solid, each of which is represented by a single tight binding function $|\Phi_j(\mathbf{k})\rangle$. Thus

$$|\Psi_t(\mathbf{k})\rangle = \sum_{\mathbf{K}} C_t(\mathbf{k}, \mathbf{K})[\,|\mathrm{PW}(\mathbf{k} + \mathbf{K})\rangle - \sum_j \langle \Phi_j(\mathbf{k})|$$

$$\times \mathrm{PW}(\mathbf{k} + \mathbf{K})\rangle|\Phi_j(\mathbf{k})\rangle] \tag{4}$$

with

$$\Phi_j(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N}} \sum_\mu e^{i\mathbf{k}\cdot\mathbf{R}_\mu} U_j(\mathbf{r} - \mathbf{R}_\mu). \tag{5}$$

In (5) $\mathbf{R}_\mu$ is a direct lattice vector and U_j is the jth atomic core state. The latter, separated into a radial and an angular part is expressed in standard notation by

$$U_{nlm}(\mathbf{r}) = \frac{P_{nl}(r)}{r} Y_{lm}(\theta, \Phi),\tag{6}$$

where the Y_{lm} functions are the standard spherical harmonics. The function $P_{nl}(r)$ is normalized as follows,

$$\int_0^\infty P_{nl}^2(r)\,\mathrm{d}r = 1.\tag{7}$$

This briefly describes the formalism of obtaining energy and wave functions in the variational procedure using model potential. In the next sub-section we briefly describe the procedure that determines the temperature dependence of the model potential.

2.1 *Temperature-dependence of model potential*

In metals, the Fourier integral of pseudo-potential factorises into two parts; the structure factor and the form factor. The former is a function of the lattice co-ordinates alone while the latter is independent of the lattice co-ordinates. It is this separation which made it possible for Kasowski [3] to express the Fourier integral of the pseudo-potential at temperature T in terms of the corresponding quantity at $T = 0$ K by the simple relation

$$\langle \mathbf{k} + \mathbf{K}| V_m |\mathbf{k}\rangle_T = \langle \mathbf{k} + \mathbf{K}| V_m |\mathbf{k}\rangle_0\, \mathrm{e}^{-W_0(\mathbf{K},T)},\tag{8}$$

where the function $\exp(-2W_0)$ is the usual Debye–Waller [3] factor. The function W_0 which depends on the frequencies $\omega(\mathbf{q}, s)$ of the phonon spectrum of the lattice is given [3] by

$$W_0(\mathbf{K}, T) = \frac{1}{2}\sum_{q,s} \frac{\hbar}{2\,\mathrm{MN}\,\omega(\mathbf{q}, s)} (2\bar{n}(q, s) + 1)|\mathbf{K}, \varepsilon(\mathbf{q}, s)|^2,\tag{9}$$

where the sum is taken over all the branches labelled by s and the wave vectors $\mathbf{q}$ in BZ. $\varepsilon(\mathbf{q}, s)$ is the polarization vector of the phonon in the mode $(\mathbf{q}, s)$, $\bar{n}(\mathbf{q}, s)$ is the average number of phonons in this mode and M is the mass of an atom in the lattice.

In order to evaluate W_0 it is essential to have phonon spectrum of the lattice at the given temperature. In the absence of the phonon spectrum for the discrete lattice, it is a reasonably good approximation to evaluate the sum in (9) using the phonon spectrum in Debye model. In the latter model, W_0 takes the form [10]

$$W_0(\mathbf{K}, T) = \left(\frac{3\hbar^2}{2Mk_B\theta_D}\right)K^2\left(\frac{T}{\theta_D}\right)^2 \int_0^{\theta_D/T} \left(\frac{1}{\mathrm{e}^x - 1} + \frac{1}{2}\right) x\,\mathrm{d}x,\tag{10}$$

where k_B is the Boltzmann constant and θ_D is the Debye temperature. Using the available Debye temperature, the integral in (10) can be evaluated for any desired temperature T. We wish to remark here that the relation in (8) which was derived for pseudo-potential holds for model potential as well.

For Sc, the phonon spectrum for the discrete lattice is not available. Hence the phonon spectrum from Debye model has been used in the present work to evaluate

$W_0(\mathbf{K}, T)$. Using (8) the Fourier integral of model potential at temperature T_2 is expressed in terms of those at T_1 as

$$\langle \mathbf{k} + \mathbf{K} | V_m | \mathbf{k} \rangle_{T_2} = \langle \mathbf{k} + \mathbf{K} | V_m | \mathbf{k} \rangle_{T_1} e^{-[W_0(\mathbf{K}, T_2) - W_0(\mathbf{K}, T_1)]}. \tag{11}$$

For Sc, the form factors are available [9] at $T_1 = 293$ K and using these the values at $T_2 = 11$ K can be calculated from (11) with W_0 determined in (10).

The band structure calculation described in §2·1 may be repeated with the temperature dependent model potential discussed above for obtaining energy and eigen functions at the desired temperatures. This makes it possible to determine the Fermi energy and hence the distribution of electrons in Fermi-volume. The latter contributes to EFG. In the following sub-section we derive the expression for the field gradient.

2.2 *Electric field gradient*

Once the true wave functions $\Psi_t(\mathbf{k}, \mathbf{r})$ of all the occupied band states in the full BZ are determined, the field gradient tensor which reduces to a single component, namely, the principal z component for hcp lattice is evaluated using the relation [11],

$$q_{el} = -\sum_{t, \mathbf{k}} \int \Psi_t^*(\mathbf{k}, \mathbf{r}) \frac{3\cos^2\theta - 1}{r^3} [1 - \gamma(r)] \Psi_t(\mathbf{k}, \mathbf{r}) d^3 r, \tag{12}$$

where the sum is taken over all the occupied bands t at the $\mathbf{k}$ points in the BZ. The function $\gamma(r)$ is the radially-dependent antishielding factor [12, 13] which accounts for the distortion of the core states of the atom in question by the nuclear quadrupole moment and the remaining charge distribution in solid. r and θ refer to the nucleus in question as the origin and the crystal C-axis as the Z-direction. The negative sign before the sum in (12) is a consequence of the negative charge on electron.

Using (4) in (12) and carrying out a considerable amount of algebra, we obtain the final expression for q_{el} as

$$q_{el} = \frac{192\pi}{\Omega} \left(\frac{16\pi}{5} \right)^{1/2} \sum_{\mathbf{K}} \omega(\mathbf{k}) \sum_t \sum_{\mathbf{K}, \mathbf{K}'} C_t^*(\mathbf{k}, \mathbf{K}) C_t(\mathbf{k}, \mathbf{K}')$$

$$\times S(\mathbf{K}' - \mathbf{K}) D(|\mathbf{K}' - \mathbf{K}|) Y_{20}(\mathbf{K}' - \mathbf{K})$$

$$- \frac{1536}{\Omega} \left(\frac{\pi^5}{5} \right)^{1/2} \sum_{\mathbf{k}} \omega(\mathbf{k}) \sum_t \sum_{\mathbf{K}, \mathbf{K}'} C_t^*(\mathbf{k}, \mathbf{K}) C_t(\mathbf{k}, \mathbf{K}') S^*(\mathbf{K}) S(\mathbf{K}')$$

$$\times \sum_{nlm} \sum_{n'l'm'} (i)^{l' - l} Y_{lm}(\mathbf{k} + \mathbf{K}) Y_{l'm'}^*(\mathbf{k} + \mathbf{K}') I(nl, |\mathbf{k} + \mathbf{K}|) I(n'l', |\mathbf{k} + \mathbf{K}'|)$$

$$\times F(nl, n'l') \langle lm | 20 | l'm' \rangle$$

$$+ \frac{3072}{\Omega} \left(\frac{\pi^4}{5} \right)^{1/2} \sum_{\mathbf{k}} \omega(\mathbf{k}) \sum_t \sum_{\mathbf{K}, \mathbf{K}'} C_t^*(\mathbf{k}, \mathbf{K}) C_t(\mathbf{k}, \mathbf{K}')$$

$$\times S(\mathbf{K}') S^*(\mathbf{K}) \sum_{\substack{nlm \\ l'm'}} (i)^{l - l'} Y_{lm}^*(\mathbf{k} + \mathbf{K}') Y_{l'm'}(\mathbf{k} + \mathbf{K})$$

$$\times I(nl, |\mathbf{k} + \mathbf{K}'|) H(nl, l', |\mathbf{k} + \mathbf{K}|) \langle l'm' | 20 | lm \rangle \tag{13}$$

where $\omega(\mathbf{k})$ is the weighting factor assigned to the sample $\mathbf{k}$ point in the BZ, $S(\mathbf{K})$ is the structure factor and i is the imaginary number $\sqrt{-1}$. The symbols I, F, H and D stand for the radial integrals,

$$I(nl, |\mathbf{k} + \mathbf{K}|) = \int_0^\infty P_{nl}(r) j_l(|\mathbf{k} + \mathbf{K}|r) r \, dr, \tag{14}$$

$$F(nl, n'l') = \int_0^\infty P_{nl}(r) P_{n'l'}(r) \frac{[1 - \gamma(r)]}{r^3} dr, \tag{15}$$

$$H(nl, l', |\mathbf{k} + \mathbf{K}|) = \int_0^\infty P_{nl}(r)(r) j_{l'}(|\mathbf{k} + \mathbf{K}|r) \frac{1 - \gamma(r)}{r^2} dr, \tag{16}$$

$$D(|\mathbf{K}' - \mathbf{K}|) = \int_0^\infty j_2(|\mathbf{K}' - \mathbf{K}|r)[1 - \gamma(r)] \frac{1}{r} dr, \tag{17}$$

where j_l is the spherical Bessel function of order l.

The notation $\langle l_1 m_1 | l_2 m_2 | l_3 m_3 \rangle$ stands for angular integral

$$\langle l_1 m_1 | l_2 m_3 | l_3 m_3 \rangle = \int Y_{l_1 m_1}^*(\theta, \Phi) \, Y_{l_2 m_2}(\theta, \Phi) \, Y_{l_3 m_3}(\theta, \Phi) \sin \theta \, d\theta \, d\Phi. \tag{18}$$

The first, second and third $\mathbf{k}$-sums in (13) give contributions from the pure plane wave (PW–PW), the tight binding (TB) and the hybrid (plane wave-tight binding and tight-binding-plane wave) part of Ψ_t respectively.

The contribution to EFG from the lattice ions, evaluated in point-ion approximation [2], is given by

$$q_{latt} = Z(1 - \gamma_\infty)[0{\cdot}0065 - 4{\cdot}4584(c/a - 1{\cdot}633)]/a^3, \tag{19}$$

where a and c are the lattice parameters of hcp lattice, Z is the valency of atom and γ_∞ is the Sternheimer antishielding factor [13]. The contribution, q_{latt} at different temperatures can be computed from (19) by using the lattice parameters a and c at the corresponding temperatures.

3. Results and discussion

The results of EFG in scandium evaluated at 293 K have been published before [7, 8]. In the present work we have followed the same procedure as in the previous work [7, 8] but with the temperature-dependent model potential so that we have now results of EFG both at 293 K and 11 K for comparison. Since the procedure has been discussed in great detail in our previous work [7, 8], we shall briefly deal here only with the salient features of the present work leaving the details to the previous work [7, 8].

In Sc the states $1s$ through $3p$ have been treated as core states, each of which is represented by a single TB function. The atomic core functions used for this purpose are the Hartree-Fock functions of Clementi [14]. Energy and wave functions are calculated at 144 representative $\mathbf{k}$ points in the 1/24th irreducible part of the BZ. For this purpose the triangular prism denoting the irreducible part has been divided into nine equal parts by slicing it along the C-axis in perpendicular direction. Each part is further

divided into 16 equal-volume sub-prisms. The centroid of each sub-prism is chosen as the representative k-point at which band calculations are carried out. To each k-point a weighting factor $\omega(\mathbf{k})$ in proportion to the volume it represents is assigned. For Sc the volumes being equal, the weighting factors are also equal for all the 144 k-points. This choice amounts to using 3456 (144 × 24) k-points in the full BZ.

At each k-point the model wave function χ_t has been expanded in 23 plane waves corresponding to the shortest 23 wave vectors $|\mathbf{k} + \mathbf{K}|$ for that k-point. This makes the size of the matrix 23 × 23. With this, choice energy and eigen functions are found well converged. The energies of occupied band states have converged to within 0·001 Ry. The band calculation is carried out at both 293 K and 11 K. For the latter temperature, model potential is evaluated using the values at 293 K in (11) after calculating W_0 in Debye model. It may be noted here that W_0 obtained in this model will be a good approximation to its exact value. The latter could not be evaluated as the phonon spectrum of Sc lattice is not available in the literature.

The results of band calculation at 293 K are compared with those of the other works [5]. There is overall agreement between the two calculations. Details of comparison are given in the previous work [7, 8]. Fermi energy is determined by counting the number of occupied band states at all the representative k-points such that the total number of conduction electrons are accommodated. This procedure is repeated for both the temperatures. It is found that the Fermi energy changes slightly, but the number of occupied states at each sample k-point remains the same at both the temperatures. This is so because the change in energies of band states due to variation of temperature in the range considered is so little that it does not affect the distribution of Fermi-volume electrons. It does however bring about changes in the character of the wave function. With a view to examining the latter, we have compared the coefficients $C_t(\mathbf{k}, \mathbf{K})$ of occupied bands at two temperatures at some of the sample k-points. We find a very small change in their values. This analysis suggests that the variation of the model potential with temperature is perhaps not significant in the given temperature range. In order to see how much is the change in the form factor due to the temperature variation, we have calculated the ratio of $\langle \mathbf{k} + \mathbf{K} | V_m | \mathbf{k} \rangle$ at 11 K to its value at 293 K. This ratio, as can be seen from (11) is equal to $\exp[W_0(\mathbf{K}, 11°) - W_0(\mathbf{K}, 293°)]$, which in view of (10) turns out to be $\exp(0·009571 K^2)$ in case of Sc. The latter is less than 1·01 for the largest K used in the calculation. This shows that model potential differs less than by 1% when the temperature is changed from 293 K to 11 K. This is indeed a very small change, which explains why there is marginal change in the character of wave function and no change in the distribution of Fermi-volume electrons. This analysis also leads one to expect a small change in the electron contribution to EFG due to change of temperature from 293 K to 11 K.

We now discuss the field gradient results. Since $\gamma(r)$ for Sc is not available in the literature, we have assumed it as zero while evaluating integrals in (15)–(17). This assumption was also made in our previous work [7, 8] while evaluating EFG in Sc at 293 K. This assumption, as explained in our previous work [7, 8], would significantly affect only the pure plane-wave (PW–PW) part of the contribution to EFG. Its effect on the contribution from the non-plane wave part of Ψ_t is expected to be negligible for reasons explained in the previous work [7, 8]. Although $\gamma(r)$ is put equal to zero, an estimation for the shielded PW–PW contribution has been made in the same way as reported in the previous work [7, 8]. The shielded PW–PW contribution is obtained by enhancing the unshielded ($\gamma(r) = 0$) value by a factor $(1 - \gamma_\infty/2)$. The validity of this assumption is discussed in [7].

The integrals in (14)–(17) are evaluated by generating each integrand at 201 mesh points chosen in a log scale,

$$r_n = r_1 e^{(n-1)h}, \tag{20}$$

where the mesh size $h = 0.045$ au and $r_1 = 0.00237$ au. The farthest distance up to which integration has been carried out has the value $r_{201} = 19.21089$ au. The values of the angular integrals in (18), on the other hand, are taken from the tabulated values [15] for the allowed combinations of angular momentum. The rules of addition of angular momentum suggest that the only allowed combinations in Sc, where there are no d cores, are $s - d$, $p - p$ and $p - f$ in spectroscopic notation. The contributions to EFG from these terms are evaluated separately, with a view to finding their relative importance. In addition to these, there is a contribution, referred to 'distant' contribution [7] which arises from the $l = 0$ component of electronic charge distribution located on lattice sites other than the one in question. The lattice contribution to EFG has been calculated using (19) for the two temperatures. The electronic and lattice contributions at the two temperatures are summarized in table 1. In the present work as well as in the previous calculation [7, 8] the value of γ_∞ used is -23.104. It refers to the solid-state value rather than the free-ion value and is taken from the work of Schmidt *et al* [16].

From table 1, it is seen that the change in the electronic contribution due to temperature variation is indeed small as expected. This is due to the small change in model potential in the given temperature range. At each temperature, it is noticed that the $p - p$ contribution has the largest magnitude. This is understandable because the p-states give the most asymmetric charge distribution. Comparing the individual components of electronic contribution at the two temperatures, one notices from table 1 that the values at 293 K are systematically lower in magnitude than those at 11 K. This may be explained by the reduction of the strength of potential. In the Kasowski formalism [3], we have seen before that the Fourier integrals of model potential at 11 K are larger than those at 293 K by the factor $\exp(0.009571 K^2)$ in Sc. This suggests that potential at 11 K is stronger than at 293 K. As a result the electron distribution at 293 K is more free-electron-like than at 11 K. Accordingly, s-character of charge distribution increases at the expense of the more important p character at 293 K and causing a reduction in the magnitude of EFG. The lattice contribution to EFG, on the other hand, changes more significantly than the electronic contribution and this results primarily from the change in the c/a ratio of the lattice due to temperature variation. Adding q_{el} to q_{latt}, the net EFG comes to -8.009×10^{13} esu/cm^3 and -3.756×10^{13} esu/cm^3 at 293 K and 11 K respectively. Results from experiment [17] as well as from other work [18] are available only at 293 K. The experimental result [17] of which the sign is undetermined is: $|q| = 13 \times 10^{13}$ esu/cm^3. The result from Blaha *et al* [18] who have used the linearized-augmented plane wave procedure is $q = 32 \times 10^{13}$ esu/cm^3. As far as the magnitude of EFG is concerned, the present result is more close to experiment [17] than those of Blaha *et al* [18]. But as to the sign of EFG, nothing can be said conclusively until the sign of experimental EFG is determined. The present result is likely to improve if $\gamma(r)$ appropriate to solid state is used in the calculation instead of estimating its effect as has been done in the present work.

It is suggested that attempts be made on the experimental side to measure the EFG in Sc at 11 K so that it would offer a good test for the accuracy of the present result.

Table 1. Electric field gradients in hcp scandium metal at 11 K and 293 K. EFG's are expressed in units of 10^{13} esu/cm^3.

| T | q_{latt} | Present work q_{el} | | | | | Total | | Other work* | Expt. |
		PW–PW shielded	$s-d$	$p-p$	$p-f$	dist	q_{el}	Net q	Net q	$|q|$
11	128·390	−6·200	−4·854	−119·643	−1·346	−0·103	−132·146	−3·756	–	–
293 K	122·176	−5·724	−4·808	−118·231	−1·324	−0·098	−130·185	−8·009	32·0	13·0

*Blaha *et al* [18]

4. Conclusions

Electric field gradients in scandium metal calculated at two temperatures show that the relative change in the electronic contribution is much less than the change in the lattice contribution. The net EFG is found to be $-3 \cdot 756 \times 10^{13}$ esu/cm^3 and $-8 \cdot 009 \times 10^{13}$ esu/cm^3 at 11 K and 293 K respectively. This agrees reasonably well with the available experimental result. For a more meaningful comparison, it is suggested that not only the sign of EFG be determined in experiment but also measurement of EFG at other temperatures including 11 K be made.

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