Augmented Plane Wave Study of Electric Field Gradients in Non-cubic Metals*

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The electric field gradient (EFG) in body-centered tetragonal Indium metal and hexagonal closed packed Beryllium metal is calculated on the basis of a full potential scalar relativistic augmented plane wave procedure. The various contributions to the EFG in simple metals are discussed. The total EFG in In metal found theoretically is equal to $q_{\text{theor}} = 2.67 \times 10^{21}\,\text{Vm}^{-2}$. This value agrees well with the experimental data. Using the quadrupole moment Q deduced from the hyperfine splitting of the muon X-ray spectra one gets $q_{\text{exp}} = 2.46 \times 10^{21}\,\text{Vm}^{-2}$. The valence electrons of Indium give a direct contribution of $q_{\text{el}} = 2.72 \times 10^{21}\,\text{Vm}^{-2}$, whereas the direct ionic contribution q_{ion} is much smaller and has opposite sign: $q_{\text{ion}} = -0.01 \times 10^{21}\,\text{Vm}^{-2}$. There is a small net shielding contribution of $q_{\text{sh}} = -0.03 \times 10^{21}\,\text{Vm}^{-2}$ to the EFG composed of the ionic contribution $q_{\text{sh, ion}} = -0.39 \times 10^{21}\,\text{Vm}^{-2}$ and the valence electron contribution $q_{\text{sh, ve}} = 0.36 \times 10^{21}\,\text{Vm}^{-2}$.

I. Introduction

In studies of nuclear quadrupole interactions the use of radiative techniques [1–4] in addition to conventional resonance techniques [5] often allows one to determine not only the signs of the nuclear quadrupole coupling constants but also their values and to measure the asymmerty parameters for the field-gradient tensors at the nuclei in perfect and imperfect metals. The advances in the corresponding theory have been described in recent reviews [6, 7].

A particularly challenging problem for theory is to explain the experimental nuclear quadrupole interaction data in Indium metal, where the structure is body-centered tetragonal, with the c/a ratio close to unity [8] ($a = 455.55$ pm, $c/a = 1.0831$), i.e. the structure of close to body-centered cubic with zero electric field-gradient (EFG). This closeness to cubic character makes an accurate evaluation of contributions to the EFG from different parts of the Brillouin zone (BZ) very critical because one expects strong cancellations of contributions from different parts of the BZ.

In this article, we present the results of our calculations on the EFG in Indium by the self-consistent augmented plane wave (APW) method using a non-spherical potential around the nuclei [9]. In a similar earlier investigation on Be metal [10] we used the muffin-tin approximation [11]. The influence of the non-sphericity on the EFG has been considered in recent work [12, 13] by the linearized APW procedure [14]. To see the differences in the EFG within the APW muffin-tin and non muffin-tin approximations and the APW and linearized APW procedures, we have recalculated the EFG in Be metal, which has been extensively investigated theoretically [10, 12, 13, 15, 16]. Sternheimer antishielding contributions [17] to the EFG can be included in two ways. This will be discussed in some detail in the following Section.

II. Method

Electric Field Gradient (EFG)

In view of the axial symmetry of the tetragonal or hexagonal environment around each In^{3+} or Be^{2+} ion, there is no asymmetry parameter and one has only to study the EFG parameter q, representing the maximum component in the principal axis system. It is given by

$$q = q_{\text{ion}} + q_{\text{ve}} + q_{\text{sh}}, \qquad (1)$$

$$q_{\text{ion}} = \frac{Z_c e}{4 \pi \varepsilon_0} \sum_s \frac{3 \cos^2 \vartheta_s - 1}{r_s^3}, \qquad (2)$$

$$q_{\text{ve}} = - \frac{e}{4 \pi \varepsilon_0} \int \frac{\varrho_{\text{ve}}(r)(3 \cos^2 \vartheta - 1)}{r^3} \, d\tau. \qquad (3)$$

q_{ion} is the direct contribution (excluding shielding effects) of the external ionic charges (nuclei and core electrons besides the core around the nucleus considered). The quantity Z_c is the charge on these ions (e.g. $Z_c = +2$ in Be treating the 1 s electrons as core), ϑ_s is the angle between the line joining the *s*th ion and the central one (containing the nucleus under study) and the *z*-axis, and r_s is the length of that line.

q_{ve} is the contribution of the electrons which are treated as band electrons (e.g. the 2 s valence electrons in Be) and therefore are not included in q_{ion}. Here $\varrho_{\text{ve}}(r)$ is the electron density deduced by summing over all occupied one-electron states $\psi_{k,n}(r)$:

$$\varrho_{\text{ve}}(r) = \sum_{k,n}^{\text{occ.}} \varrho_{k,n}(r), \qquad (4)$$

$$\varrho_{k,n}(r) = 2 |\psi_{k,n}(r)|^2, \qquad (5)$$

where k is the wave vector and n is the band index.

q_{sh} represents the shielding effect of the core electrons around the nuclei considered. This contribution can be treated in two ways, either by perturbation theory or by incorporating the core electrons into the band structure calculation.

The first method is straightforward for ionic crystals where the theory ends up with the use of the Sternheimer antishielding factor γ_∞ [18]. For metals, the shielding effect of the ion cores can be calculated in the same manner as for ionic crystals, namely

$$q_{\text{sh,ion}} = - q_{\text{ion}} \gamma_\infty. \qquad (6)$$

However, to study the contribution of the valence electrons the perturbation approach is much more complicated [19, 20]. As the valence charge distribution is not totally external to the ionic cores, an anti-shielding function $\gamma(r)$ has to be used to determine the shielding effect due to the valence electrons [6, 21]:

$$q_{\text{sh,ve}} = \frac{e}{4 \pi \varepsilon_0} \int \gamma(r) \frac{\varrho_{\text{ve}}(r)}{r^3} \, d\tau. \qquad (7)$$

The second method to study the antishielding effect is more convenient than the perturbation approach. However, it can only be used within a full potential self-consistent field procedure. Here the net shielding contribution

$$q_{\text{sh}} = q_{\text{sh,ion}} + q_{\text{sh,ve}} \qquad (8)$$

can be calculated directly by treating the core electrons as band electrons using the same procedure as for the valence electrons described below.

It has never been investigated before whether both methods give the same answer. However, in the case of small molecules it has been shown that the direct Hartree-Fock calculation of the EFG for a nucleus inside an ion with point charges adjacent to it, and the use of γ_∞ give the same result [22]. Using the perturbation theory for metals, it has been shown for Zn and Cd [19, 20] that the antishielding due to the ionic contribution $q_{\text{sh,ion}}$, and the antishielding caused by the valence electrons $q_{\text{sh,ve}}$ are large and have opposite sign. The net antishielding effect in metals q_{sh} is found to be small compared to the total EFG [19, 20]. For example for Cd metal $q_{\text{sh}} = 0.35 \times 10^{21} \, \text{Vm}^{-2}$ (composed of $q_{\text{sh,ion}} = -3.48 \times 10^{21} \, \text{Vm}^{-2}$ and $q_{\text{sh,ve}} = 3.83 \times 10^{21} \, \text{Vm}^{-2}$) as compared to the total EFG found theoretically $q_{\text{theor}} = 8.98 \times 10^{21} \, \text{Vm}^{-2}$ [19, 20]. Thus the shielding effect contributes only 4% to the total EFG. Studying q_{sh} directly by a full potential linearized APW band structure calculation one gets a net shielding for Cd metal of 1% [13]. Therefore both methods, perturbation approach and band structure procedure for dealing with core electrons, give at least the same order of magnitude for the shielding effects. In the present work this is also found for Indium metal, see below.

In earlier papers, see e.g. [6], the ionic contribution is mostly defined by the sum of q_{ion} and $q_{\text{sh,ion}}$,

$$q_{\text{ion,total}} = q_{\text{ion}} + q_{\text{sh,ion}}, \qquad (9)$$

that is the given values for the ionic contribution to the EFG ($q_{\text{ion,total}}$) include the antishielding effect. In the present work, however, only the direct part of the ionic contribution q_{ion} is listed below in Tables 1 and 2.

The Crystal Potential

To construct the crystal potential for the APW calculation, the crystal is subdivided into two regions, non overlapping spheres around the nuclei and the region outside these spheres. Inside the spheres the potential is expanded in spherical harmonics (or crystal harmonics) $Y_{l,m}$ [9],

$$V_{l,m}(r) = \sum V_{l,m}(r) Y_{l,m}(\hat{r}). \qquad (10)$$

Outside the atomic spheres $V(r)$ is approximated by a Fourier sum over the reciprocal lattice vectors K [9],

$$V(r) = \sum_K V(K) \, e^{i K \cdot r}. \tag{11}$$

Three contributions are included in $V_{l,m}(r)$ and $V(K)$: the lattice contribution of the ionic cores calculated by a method given by Nagel [23], the Coulomb contribution of the electrons deduced by solving the Poisson equation for $\varrho(r)$, and the exchange contribution which is calculated within the local density approximation [24].

In (10) and (11), $V_{l,m}(r)$ and $V(K)$ are chosen in such a way that $V_{0,0}(r)$ and $V(O)$ correspond to the spherical symmetric muffin-tin potential.

Electron Density

The wave functions $\psi_{k,n}(r)$ are expanded in the usual way [11] in terms of augmented plane waves φ_i, namely,

$$\psi_{k,n}(r) = \sum c_i \, \varphi_i(\varepsilon^0_{k,n}, r). \tag{12}$$

The $\varepsilon^0_{k,n}$ in (12) indicate that the basis functions φ_i are exact solutions of the Schrödinger equation using the muffin-tin approximation. Therefore $\psi_{k,n}$ is calculated in two steps. First the muffin-tin approximation is used (taking only $V_{0,0}(r)$ and $V(O)$ of $V(r)$) and the coefficients c^0_i and basis functions $\varphi_i(\varepsilon^0_{k,n}, r)$ are deduced variationally in a self-consistent calculation. In a second step the coefficients c_i are calculated self-consistently for the full crystal potential using the basis functions $\varphi_i(\varepsilon^0_{k,n}, r)$.

From the wave functions, the charge density $\varrho_{ve}(r)$ can be calculated according to (4) and (5). It is useful to expand $\varrho_{ve}(r)$ in the same manner as $V(r)$, as in (10) and (11). Then inside the atomic spheres the electronic contribution of q, q_{el}, is simply given by an integral over the $\varrho_{2,0}$ component:

$$q_{el} = -\sqrt{\frac{16\pi}{5}} \frac{e}{4\pi\varepsilon_0} \int \frac{\varrho_{2,0}(r)}{r} \, dr. \tag{13}$$

In recent papers [12, 13] it has been suggested that it is preferable to use the electrostatic part of $V_{2,0}(r=0)$ to obtain q. Actually the conventional procedure represented by (13) is equivalent to the latter procedure.

Summation Over the Brillouin Zone

It is known from the literature that the calculated EFG can be sensitive to the chosen mesh points k_m of

allowed k vectors in the BZ. To determine the total electron density and the total EFG we have used the tetrahedral method. Taut and Lehmann [25] have given an algorithm to evaluate surface integrals

$$A_F = \int_F A(k) \, dS, \tag{14}$$

where $A(k)$ is the physical property under study and F is for example the Fermi surface. This algorithm is expanded to evaluate volume integrals over the occupied (Fermi) volume V_F^* of BZ:

$$I_{V_F^*} = \int_{V_F^*} A(k) \, dV^*. \tag{15}$$

We have used this method to calculate the electron density and the EFG q_{el}. For such a calculation, $A(k) \equiv \varrho_{k,n}$ for the electron density and $A(k) \equiv q_{el}^{(k,n)}$ for q_{el} in (13). The entity $\varrho_{k,n}$ is the electron density $2|\psi_{k,n}|^2$ corresponding to a particular electronic state $\psi_{k,n}$, and $q_{el}^{(k,n)}$ is the contribution to q from the same state, obtained by substituting the contribution $\varrho_{2,0}(r)$ from $\varrho_{k,n}(r)$ in (13).

III. Results

Be

A crucial test for the confidence in the computational procedure is the study of the EFG in Be metal. The c/a ratio of hcp Be metal is close to the ideal value and one finds [6, 10, 16] a strong cancellation of different contributions to the EFG. In this section the convergence of the EFG with respect to the chosen potential and with respect to the number of mesh points k_m in the BZ is discussed. The convergence with respect to the choice of the basis set expansion has been considered in a previous paper [10].

First, the convergence with respect to the number of mesh points in k space shall be considered. The mesh points k_m are chosen to be equally spaced parallel to the basis vectors of the reciprocal lattice as in earlier work [10]. To avoid oscillations in the calculated EFG with increasing number of k_m it is necessary to choose the mesh width in such a way that all corners of the irreducible part of the BZ become mesh points of the grid. With this choice of mapping a convergence better than 2 per cent is reached for q_{el} for about 300 k_m in the irreducible part of the BZ. The results in Table 1 correspond to a calculation using the tetrahedral method on the basis of a larger number, namely, 370 k_m in the irreducible part of the BZ. However, the

actual integration is carried out over the entire rather than the irreducible part of the BZ [26].

In Table 1 our results for the EFG in Be metal are summarized. The calculations were carried out using lattice parameters $a = 228.66$ pm and $c/a = 1.567$. To test the convergence with respect to the potential, the data are given for three different crystal potentials, a) the muffin-tin potential, b) an intermediate muffin-tin potential involving a full potential with both r and directional dependence inside the atomic spheres (see

Table 1. List of various contributions of the EFG in units of 10^{21} V m^{-2} in Be metal calculated for three different crystal potentials.

	Muffin-tin potential	Full potential inside the muffin-tin-sphere	Full potential
Valence electron contribution			
1st band	0.4493	0.4447	0.4374
2nd band	−0.5202	−0.5318	−0.5440
3rd band	0.0105	0.0114	0.0108
Sum (q_{el})	−0.0604	−0.0757	−0.0958
Ionic contribution (q_{ion})[a]	0.0711	0.0711	0.0711
Total (q)	0.0107	−0.0046	−0.0247
Experiment (q_{exp})		±0.042[b]	

[a] Ref. [27].
[b] Based on $Q = 0.054$ barn and experimental coupling constant in the metal from [29, 30].

Table 2. Various contributions to the EFG in bct In metal.

	EFG in 10^{21} V m^{-2}	EFG in 10^{13} esu cm^{-3}
Valence electron contribution		
1st band	2.090	69.66
2nd band	1.186	39.53
3rd band	−0.554	−18.47
Sum (q_{el})	2.722	90.72
Ionic contribution (q_{ion})	−0.015	−0.49
Core electron contribution (q_{sh})[a]	−0.034	−1.12
Total theoretical result (q)	2.673	89.11
Experimental result (q_{exp})[b]	2.46[b]	82.08[b]

[a] Listed is the band structure result. From the perturbation approach we found:
$q_{sh, ion} = -0.394 \times 10^{21}$ V m^{-2}; $q_{sh, ve} = 0.364 \times 10^{21}$ V m^{-2}; $q_{sh} = -0.030 \times 10^{21}$ V m^{-2}.
[b] Based on $Q = 0.76$ barn derived in Section III and the experimental coupling constant in the metal from [32].

(10)) but a constant one outside the atomic spheres, and c) a full potential in both regions.

In Table 1 the ionic contribution (nuclei and 1 s core) q_{ion} [27] and the valence electron contribution q_{el} are listed separately. The shielding of the 1 s core electrons is neglected because γ_∞ is small for Be^{2+} ($\gamma_\infty = 0.2$ [28]) and because of the cancellation of $q_{sh, ion}$ and $q_{sh, ve}$, see Section II. The experimental result is also listed for comparison. The magnitude of the experimental value of q is obtained using the average values of the measured ^{9}Be quadrupole coupling constants from [29] and [30] and the value of $Q = 0.054 \times 10^{-24}$ cm^2 [31], where a many-body calculation of the EFG at the beryllium atom in the excited $1 s^2 2 s 2 p (^3P)$ state was carried out.

One sees from Table 1 that there is strong cancellation both in the contributions to q_{el} from different bands and between q_{ion} and q_{el} leading to very small results for the total EFG's in all three cases. On comparing the muffin-tin and non muffin-tin results, one sees that the non muffin-tin results for the total q for potential c) is closer to the experimental one as has also been found [12] by the linearized APW procedure.

The intermediate muffin-tin potential b) leads to results for both q_{el} and q between the results for a) and those for the full potential c), as expected. It is interesting, however, that the results for potential b) are significantly different for that for c), indicating that it is not sufficient to use the full potential within the atomic spheres only.

In

The results for the EFG in bct Indium metal are summarized in Table 2. In the following the various contributions to the EFG shall be considered.

The main contribution to the EFG in Indium metal arises from the electrons in the valence bands (corresponding to the 5 s and 5 p electrons of the Indium atom). Since there is only one atom per unit cell there are three electrons occupying the valence bands. These are distributed over the 1st to 3rd electronic bands according to the occupation numbers $n_1 = 2.000$, $n_2 = 0.990$ and $n_3 = 0.010$. The band structure of these electron states is given in Figure 1.

The contributions to the EFG are positive for the first two bands and negative for the 3rd band (see Table 2). The sum of the contributions of the three

bands leads for In metal to a total positive contribution of $q_{el} = 2.72 \times 10^{21}$ Vm^{-2}. In contrast to the results for Be, this contribution is mainly caused by the non cubic symmetry of the Fermi volume rather than the non sphericity of the crystal potential. This can be seen by taking only the muffin-tin component of the self-consistent potential. Using the muffin-tin potential one gets $q_{el} = 2.65 \times 10^{21}$ Vm^{-2}, which is close to the full potential result given above.

The ionic contribution of the external ionic cores of charge $+3$ [33] is opposite in sign to the valence electron contribution q_{el} and is distinctly smaller in magnitude. Thus, there is no significant cancellation between q_{el} and q_{ion} as found for Be metal.

The contribution of the core electrons (1 s to 4 d) around the nucleus as obtained using the electronic wave-functions for the corresponding core bands is seen from Table 2 to lead to a small shielding effect of $q_{sh} = -0.03 \times 10^{21}$ Vm^{-2}.

Using instead the perturbation theory, the following results are found: The ionic contribution to the EFG is taken from [33], $q_{ion} = -0.0146 \times 10^{21}$ Vm^{-2}; using an antishielding factor of $\gamma_\infty = -26.95$ one gets [33] $q_{sh, ion} = -0.394 \times 10^{21}$ V^{-2}. Then, the total ionic contribution according to (9) is equal to $q_{ion, total} = -0.409 \times 10^{21}$ Vm^{-2}. To determine the valence electron contribution to the shielding effect the antishielding function for In^{3+} is taken from [34]. Performing the integration (7) one finds $q_{sh, ve} = 0.364 \times 10^{21}$ Vm^{-2}. The total shielding effect results in $q_{sh} = q_{sh, ion} + q_{sh, ve} = -0.03 \times 10^{21}$ Vm^{-2}, which is close to the result gained from the band structure procedure.

Finally, the total EFG found theoretically ($q_{theor} = +2.67 \times 10^{21}$ Vm^{-2}) shall be compared with the experimental result. Experimentally, the sign of the EFG is uncertain [35, 36] and our result favors a positive sign in Indium metal. Concerning the magnitude of q, the deviation of the experimental value from the measured quadrupole coupling constant requires a knowledge of Q of the ^{15}In nucleus. From the quadrupole coupling constant associated with the muonic atom involving a negative muon captured in a hydrogenic $2 p_{1,2}$ state around the Indium nucleus it has been found that the use of $Q = 0.834$ barns [37] leads to an overestimation of the experimental coupling constant of about 9%. This lets expect a value of Q of 0.76 barns. Such an estimation is in keeping with the reduction which for Al atom [38], which has a similar valence configuration as Indium, was applied to the value of 0.81 barns [39] obtained from atom beam
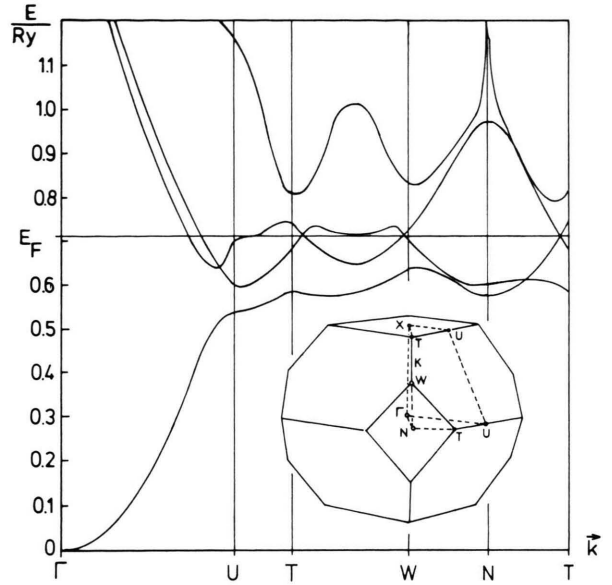

Fig. 1. Band structure of the valence electron states of Indium metal.

results on Indium atom after consideration of the Sternheimer antishielding effect. Using $Q = 0.76$ barn one gets an experimental value $q_{exp} = 2.46 \times 10^{21}$ Vm^{-2}. This value is quite close to the theoretical result, being about 8% lower.

IV. Discussion

First we discuss the results for Be metal. In an earlier paper [10], by the non self-consistent muffin-tin APW procedure we had found $q_{el} = -0.026 \times 10^{21}$ Vm^{-2}. The difference between this result and the muffin-tin result $q_{el} = -0.060 \times 10^{21}$ Vm^{-2} presented here is mainly caused by the use of the non self-consistent procedure in the earlier work and by differences in the summation over k space. The tetrahedral method [25] was not used in the earlier work [10], and because of the strong cancellation between the contributions of different bands, see Table 1, a difference of nearly a factor of 2 results from the two methods of summing over k space.

It should be noted that it is really the dependence of q_{el} on the potential that is theoretically pertinent since q_{ion} is independent of the choice of the potential. On comparing the net q in Table 1 for the three potentials, a much too extreme dependence on the potential is

observed which does not have any general significance, since this dependence is a consequence of the special situation for this metal, the strong cancellation between q_{ion} and q_{ei}. In fact the q_{el} in Table 1 for the muffin-tin potential a) is about 60 per cent of that for c). Within the linearized APW procedure, however, the muffin-tin result for q is almost 18 times larger [13] than the non muffin-tin result, in contrary to our results. We do not understand this discrepancy for the following reason.

There are two effects which contribute to q_{el}. First, the non-cubic shape of the Fermi surface leads to a finite EFG on summing over the occupied states. This is the only effect which can be evaluated within the muffin-tin approximation. The second contribution results from the non-sphericity of the potential around the nucleus under study. This effect is taken into account within the full potential calculation. Within the APW approximation used in the present work, both effects, the non-cubic Fermi surface and the non sphericity of the potential result in contributions to the EFG which have the same sign, and therefore q_{el} for the full potential is expected to be larger than q_{el} for the muffin-tin approximation.

Comparing our total result in Table 1 for Be metal $q_{theor} = -0.025 \times 10^{21} \, Vm^{-2}$ using the full potential c) with the result $-0.066 \times 10^{21} \, Vm^{-2}$ [12] deduced recently by the linearized APW procedure [14] one sees that the experimental result of $q_{exp} = \pm 0.042 \times 10^{21}$ Vm^{-2} is between the two theoretical results, both theoretical methods predicting the same (negative) sign for the EFG in Be metal.

Thus, the results of the present investigation for Beryllium indicate that even the complete self-consistent APW procedure using a full potential with directional dependence and an accurate method like the tetrahedral method for summing over k space in calculating the electronic contribution to q_{el} does not give exact agreement between theory and experiment. However, the importance of using a very sophisticated method to evaluate the EFG is particularly accentuated for Beryllium due to the various strong cancellations in the contributions to the EFG in this metal, between various parts of the BZ and different bands for q_{el} and between q_{ion} and q_{el}.

As for the results in Indium metal, the theoretical value from Table 2 as discussed in Section III agrees with experiment within 8%. This satisfactory agreement between experiment and theory leads us to expect that the negative sign obtained from the theory is correct. It is hoped that the uncertainty in the experimental results can be resolved in the future.

After our work was completed, we learnt about a value of $q_{theor} = 2.07 \times 10^{21} \, Vm^{-2}$ obtained by linearized APW calculations [40]. This value is about 25% lower than our value. It is possible that this difference could be partly associated with the use of a smaller c/a ratio of 1.076 and differences in the flexibility of the basis functions used for the calculations.

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