The derivation of pseudoatom information in germanium from total-energy calculations

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Abstract. It is shown how information about the pseudoatom in germanium can be derived from knowledge of the charge density gained from total-energy calculations. The charge densities of the equilibrium crystal and of a crystal where the ions in each cell have been moved by small, equal amounts δR in opposite directions (the LTO mode at Γ) are used to derive the Fourier components of the pseudoatoms at reciprocal lattice vectors. The total-energy calculations are carried out by solving the Kohn–Sham equations within the local density approximation. The harmonic contribution to the Fourier components of the change in charge density is derived from total-energy calculations at two different values of δR. By using symmetry, linear equations involving the real and imaginary parts of the rigid ion and the deformation can be obtained from a total-energy calculation with just one distortion of the crystal. The parts of these linear equations involving the unknowns are linearly dependent, and the calculated results have approximately the same dependence. It is shown that any discrepancies are due to anharmonic effects. The results show that the rigid ion is atomic-like with only a small deviation from spherical symmetry, and that the deformation is significant and acts mainly on the bond charges. Contour plots of the various contributions, including the anharmonic one, in the [110]–[001] plane are drawn.

1. Introduction

The change in the electronic charge density to first order in the displacements when a phonon is present in a crystal is an important quantity. It is of particular use in calculating the electronic contribution to the dynamical matrix of a crystal (Sinha 1973). From this the phonon frequencies and modes can be calculated.

There are many methods of calculating the phonon frequencies and modes. These methods can be broadly classified as empirical approaches and *ab initio* approaches. Two well-known *ab initio* methods of calculating phonon frequencies are (Srivastava 1990):

(i) total-energy calculations (Chadi and Martin 1976, Kunc and Martin 1982).
(ii) calculation of the dielectric matrix (Van Camp *et al* 1979, Falter 1988).

Both these methods have been shown to be successful but have, in a practical sense, some limitations. For example, they both involve a lot of computation, so that (i) is only affordable at symmetry points and along symmetry directions (Srivastava and Kunc 1985, 1988, Strauch *et al* 1990) and (ii) gives more information than is necessary for

calculating phonon frequencies. Furthermore, numerical data provided by such methods are not easy to convert into many concepts with which to get physical insight.

When the effective charges are zero, the first-order change in charge density can be expressed in terms of pseudoatoms (Ball 1975, 1977). The calculation of phonon frequencies and eigenvectors can be performed if the pseudoatoms are known. Calculation of the pseudoatom† is in principal a better approach than the other methods (see above) because it involves the exact amount of information required and should provide useful physical insight. It may also be possible to understand different types of phonon behaviour in terms of different types of pseudoatom.

In this paper we outline a program (see section 2) to deduce information about the pseudoatom from total-energy calculations (TECs). In particular, for germanium we use the charge densities of the perfect crystal and of a crystal in which the ions in each unit cell move by the same amount but in opposite directions (the LTO mode at Γ), to calculate the Fourier components of the pseudoatom at reciprocal lattice vectors (RLV) g.

In the past (Falter 1988) calculation of the pseudoatom has required calculation of the dielectric matrix. Calculating the pseudoatom from TECs overcomes this problem but might seem unnecessary, as we could calculate phonon frequencies directly from the TECs. We think, however, that it is advantageous: firstly, we are interested in more than just the phonon frequencies and the pseudoatom should give more physical insight into what is going on. Secondly, there are methods of using a limited amount of pseudoatom information to deduce the pseudoatom at all values of $q + g$, either by using phenomenological models (like the moveable bond charge model of Weber (1977)) and deducing the parameters of these models from the pseudoatom information (the way to link such phenomenological models with pseudoatom theory has already been shown (Ball 1988)) or by assuming analytical expressions for the parts of the pseudoatom and fitting the parameters. The former method should give useful physical information, such as the size and shape of bond charges.

An advantage of concentrating on pseudoatoms is that they ensure that the first-order change in charge density is consistent with the symmetry of the crystal. As we show in section 5, this may not happen if the charge is calculated from the TECs without considering symmetry. Another advantage of the whole approach is that, having got an accurate, consistent first-order change, we can calculate the anharmonic effects accurately.

One of the aims of this paper is to learn about the physical nature of the pseudoatom in germanium. To this end we have drawn some contour plots (see section 6) of the changes in the electron density for the LTO(Γ) mode due to the two separate parts of the pseudoatom. Plots of the anharmonic effects are also drawn.

2. The program

The first-order change in the electronic charge density can be described by a vector field f^s. Then the electronic contribution to $D_{\alpha\beta}^{s's}(q)$, the $\alpha\beta$ element of the dynamical matrix in q-space, is given by (Ball 1987)

$$\sum_{g} (M)^{-1} \partial W_{s'}^* / \partial x_\alpha (q + g) f_\beta^s (q + g) \exp[i(q + g) \cdot (R_{s'} - R_s)] \tag{1}$$

where W_s is the pseudopotential of the ion at $R_{s'}$ in the unit cell, M is the mass, and the sum is over reciprocal lattice vectors g.

† Falter (1988) has introduced a related concept, the quasi-ion.

In a non-polar semiconductor like germanium where the effective charges are zero, the change in the electronic charge density can be expressed, to first order in the displacements of the ions from their lattice positions, as a sum of pseudoatoms (Ball 1975, 1977):

$$f_s(q + g) = (q + g)\rho_s(q + g) + b_s(q + g) \tag{2}$$

where $b_s(q + g)$ is perpendicular to $(q + g)$ and so can be written (Ball 1977)

$$b_s(q + g) = (q + g) \times B_s(q + g) \tag{3}$$

In equation (2) the first term is the electronic charge ρ that moves rigidly with the ion† (we shall call this the electronic rigid ion) and the second term b represents the deformation.

Total-energy calculations always involve the calculation of the electronic charge density, as they use the density-functional method (Srivastava 1990). As said earlier, the main aim of this paper is to use the charge density from total-energy calculations to deduce information about ρ and b.

The total electronic charge density can be written, to first order in the displacements $\delta R_s \exp(iq \cdot l)$ of the ion at $(l + R_s)$, as

$$\sum_s \left(\sum_l \rho(r - l - R_s) + (1/\tau)\delta R_s \cdot \sum_g f_s(q + g) \exp[i(q + g) \cdot r] \exp(-ig \cdot R_s) \right) \tag{4}$$

where l is a lattice vector, τ is the volume of the unit cell and the first term is the charge density of the equilibrium lattice. Thus, in principle, the vector field $f_s(q + g)$ can be got from the charge densities of TECs, provided these are available, for given $q + g$, at all possible directions of δR_s. Such calculations are unfortunately restricted to values of q in symmetry directions and then often only at high symmetry points. Nevertheless we are able to learn something about the pseudoatom from such calculations.

In germanium we write s' and s for the two ions in the unit cell i.e. $R_{s'} = -(1,1,1)a/8$. Inversion symmetry makes the calculation easier, because it yields

$$f_s(q + g) = -f_{s'}(-(q + g)) \tag{5}$$

and hence

$$\rho_s(q + g) = \rho_{s'}(-(q + g)) \qquad b_s(q + g) = b_{s'}(-(q + g)). \tag{6}$$

We now concentrate on the derivation of $\rho(g)$ and $b(g)$, for which the total energy calculation for the LO mode at Γ as well as the perfect lattice calculation is required. Let us write

$$f_s(q + g) = f_R(q + g) + if_N(q + g) \tag{7}$$

where f_R and f_N are both real, with a similar definition of ρ_R, ρ_N, b_R and b_N. As the Fourier transform $\rho_s(r)$ is a physical quantity,

$$\rho_N(-g) = -\rho_N(g). \tag{8a}$$

To ensure that $b_N(g)$ transforms in the same way as $g\rho(g)$, we have the following requirement:

$$b_N(-g) = b_N(g). \tag{8b}$$

Translational invariance (Ball 1975) requires that

$$b_s(g) \exp(-ig \cdot R_s) + b_{s'}(g) \exp(ig \cdot R_s) = 0. \tag{9}$$

Thus $b_s(g) \exp(-ig \cdot R_s)$ is purely imaginary.

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† In previous papers ρ included the ionic charge. It is more convenient to take it as the electronic charge only and we shall do this in future.

The charge density $\sigma_0(g)$ of the undistorted crystal can be written in terms of ρ_R and ρ_N:

$$\sigma_0(g) = 2[\rho_R(g) \cos(g \cdot R_s) + \rho_N(g) \sin(g \cdot R_s)]. \tag{10}$$

When the ions are displaced, the charge density depends on the displacements δR_s. In our calculations these displacements have the symmetry representation Γ and are such that

$$\delta R_s = \delta R \, 8R_s \qquad \delta R_{s'} = -\delta R \, 8R_s \tag{11}$$

with $\delta R = \pm 0.005$ and ± 0.015. For this case the charge density $\sigma(g, \delta R)$ is, to first order in δR,

$$\sigma(g, \delta R) = \sigma_0(g) + 2\delta R(8/a)R_s \cdot [g\rho_N(g) \cos(g \cdot R_s)$$
$$- g\rho_R(g) \sin(g \cdot R_s) + d(g)] \tag{12}$$

where

$$d(g) = b_R \cos(g \cdot R_s) + b_N \sin(g \cdot R_s). \tag{13}$$

3. The total-energy calculations

The Fourier coefficients $\rho(g)$ of the charge density were calculated from a self-consistent solution of the Kohn–Sham equations within the local-density approximation (Hohenberg and Kohn 1964, Kohn and Sham 1965). The interaction between valence electrons and ionic cores was simulated by the *ab initio* pseudopotential of Ge (Bachelet *et al* 1982). The electronic exchange–correlation interaction was treated within the scheme of Wigner (1937). Well converged calculations were made by expanding the pseudo-wavefunction in a plane-wave basis set with a kinetic energy cut-off of 15 Ryd.

For the undistorted Ge crystal, the Brillouin zone summation was performed by using two special k-points within the irreducible segment of the zone (Chadi and Cohen 1973). The calculated equilibrium lattice constant is 5.602 Å, which, like most other calculations based on the local-density approximation, is within 1% of the experimental value of 5.65 Å.

For the LTO(Γ) mode of atomic displacements the translational symmetry of the distorted crystal remains the same as in the undistorted structure, but the point group symmetry is reduced from O_h to D_{3d}. For this symmetry we used the calculated equilibrium lattice constant and a set of five special k-points (Yin and Cohen 1982) for the Brillouin zone summation. Calculations were found to converge well with an energy cut-off of 15 Ryd.

4. Anharmonic effects

The charge density $(\sigma(g, \delta R) - \sigma_0)$ can be explained in powers of δR for small δR,

$$\sigma(g, \delta R) - \sigma_0 = \sum_n \sigma_n(g)(\delta R)^n. \tag{14}$$

The first term in the sum represents the harmonic effects and the remainder the anharmonic effects.

The pseudoatom theory is valid to first order only and does not include the anharmonic effects. The TECs, however, calculate $\sigma(g, \delta R)$ to all orders. To calculate the pseudoatom, we must try to eliminate the anharmonic effects from the calculated values of $\sigma(g, \delta R)$. We do this in the usual way: firstly we eliminate all even-order terms in equation (14) by calculating $[\sigma(g, \delta R) - \sigma(g, -\delta R)]/2$. We then assume that all fifth- and higher order terms in equation (14) are negligible, and calculate σ_1 and σ_3 from the above quantities for $\delta R = 0.005a$ and $0.015a$. The relative values of σ_1 and σ_3 tell us how important the anharmonic effects are.

5. Symmetry and the linearity condition

Let T represent an operator of the diamond lattice which leaves the undistorted crystal invariant. Then

$$\sigma(g, T(\delta R_s)) = \sigma(T^{-1}(g), \delta R_s) \tag{15}$$

where the notation is obvious. A similar result holds for the coefficients σ_n.

This symmetry requirement produces some immediate results; for example

$$\rho_N(g) = 0 \tag{16}$$

whenever g is in an axial plane.

To calculate $\rho_R(g)$, $\rho_N(g)$ and $d(g)$, one would in general need to know $\sigma_1(g)$ for displacements in three different directions, whereas we only calculate for displacements in one direction. This difficulty is easily overcome by using the above symmetry properties of the perfect crystal. Note that, in general, there are five quantities to find, although the results for the undistorted crystal provide one result using equation (11).

To see how symmetry allows us to get the other results and because there are some interesting points to make, let us look at a particular case, the RLV $g = (2\pi/a)(5,3,1)$. In the undistorted crystal 48 RLVs can be obtained by operators T which all have the same value of σ_0. Under distortions of the form equation (11), this set breaks up into four sets, typical members of each set being $(2\pi/a)(5,3,1)$, $(2\pi/a)(-3,1,-5)$, $(2\pi/a)(-1,-5,3)$, and $(2\pi/a)(-1,5,-3)$. We thus get one equation from $\sigma_0(g)$ of the undistorted crystal and four linear simultaneous equations from the distorted TEC.

These four equations are not independent. They involve four variables d_x, d_y, d_z and $(\rho_N - \rho_R)$ and the determinant of their coefficients is zero. This lack of independence occurs at all values of g. The linear simultaneous equations from the distorted crystal always involve the same combination of ρ_R and ρ_N and are linearly dependent.

This means that the values of σ_1 should satisfy the same linear relation. It turns out that for most g the values of σ_1 calculated from the TEC approximately satisfy this relation. For example, for $g = (2\pi/a)(5,3,1)$, the results are within 0.2%.

We now present arguments to show that the discrepancies from the exact satisfaction of the relation are caused by the anharmonic effects. Although similar arguments can be presented for all g, let us look at the simple example when $g = (2\pi/a)(1,1,1)$. In this case $d(g) = 0$. There are two equations, one for g and one for g', where $g' = (2\pi/a)(1,-1,-1)$; the value of $\sigma_1(g)$ should be three times the value of $\sigma_1(g')$. There is, however, in all our calculations a slight deviation from this, a suitable measure of which is $E_r = |1 - 3\sigma_1(g')/\sigma_1(g)|$. We can work out E_r in three different ways in which the amount of anharmonicity systemically decreases. Firstly (i) we subtract the charge density of the undisturbed crystal from that of the distorted crystal with $\delta R = -0.005a$;

Table 1. Values of $E_r = |1 - 3\sigma_1(g')/\sigma_1(g)|$ calculated by different methods (i), (ii) and (iii). For explanation see text.

	Method		
	(i)	(ii)	(iii)
E_r	0.087 194	0.001 727	0.000 074 9

Table 2. The calculated values of pseudoatom quantities ρ_R, ρ_N and $d = (d_x, d_y, d_z)$, (for the ion at R_s) in units of electrons per unit cell. The rows marked * are in 10^{-2} of these units.

$(a/2\pi)g$	ρ_R	ρ_N	d_x	d_y	d_z
(1,1,1)	1.196 55	−0.120 61	0	0	0
(0,0,2)	0.785 77	0	0	0	0
(0,2,2)	0.006 71	0	−1.817 60	0	0
(1,1,3)	−0.151 08	−0.061 95	−1.644 57	−1.644 57	1.096 38
(2,2,2)	−0.148 45	−0.144 92	0	0	0
(0,0,4)	−0.185 45	0	0	0	0
(3,3,1)	0.035 08	0.112 14	−0.132 52	−0.132 52	0.795 07
(0,2,4)	−0.111 34	0	0.934 06	0.0	0.0
(2,2,4)	−0.075 91	−0.197 14	0.028 35	0.028 35	−0.028 35
(3,3,3)	−0.018 76	0.017 49	0	0	0
(1,1,5)	0.002 27	0.064 51	−0.428 80	−0.428 80	0.171 52
(0,4,4)	0.023 19	0	−0.168 23	0.0	0.0
(5,3,1)	0.014 87	−0.000 33	0.026 91	0.106 67	−0.454 54
(4,4,2)	−0.013 27	−0.001 54	−0.000 15	0.0	0.0
(0,0,6)	−0.017 76	0	0	0	0
(0,2,6)	−0.004 35	0.0	−0.103 71	0.0	0.0
(3,3,5)*	−0.0653	0.0632	0.2782	0.2782	−0.3338
(2,2,6)*	0.084 15	0.1794	−3.7688	−3.7688	2.5125
(4,4,4)*	0.3248	0.0757	0.0	0.0	0.0
(5,5,1)*	0.4718	0.0598	−1.3472	−1.3472	13.4716
(1,1,7)*	0.4642	0.0738	−8.5291	−8.5291	2.4370
(0,4,6)*	0.5267	0.0	4.4511	0.0	0.0
(6,4,2)*	0.4240	0.0778	0.9676	−0.7138	−1.3974
(5,5,3)*	0.3593	0.0997	−0.7036	−0.7036	2.3455
(7,3,1)*	0.3901	0.0400	1.2781	−3.6102	1.8835
(0,0,8)*	0.3584	0.0	0.0	0.0	0.0
(3,3,7)*	0.2421	0.0248	0.0284	0.0284	−0.0243

secondly (ii) we substract the charge densities of the crystals with $\delta R = \pm 0.005a$, and thirdly (iii) we carry out the procedure of section 3. The results are given in table 1. It can be seen that E_r gets smaller as the anharmonicity is reduced, thus confirming our hypothesis that the discrepancies are caused by the anharmonic effects. This hypothesis is further confirmed by the fact that these discrepancies are largest when the anharmonic effects are largest, e.g. for $g = (5,3,3)$.

Because the anharmonic effects were reduced (see section 4) by using an approximation, there is a small anharmonic part left in our calculation of σ_1. The linear simultaneous equations therefore do not obey the dependency conditions exactly. We need,
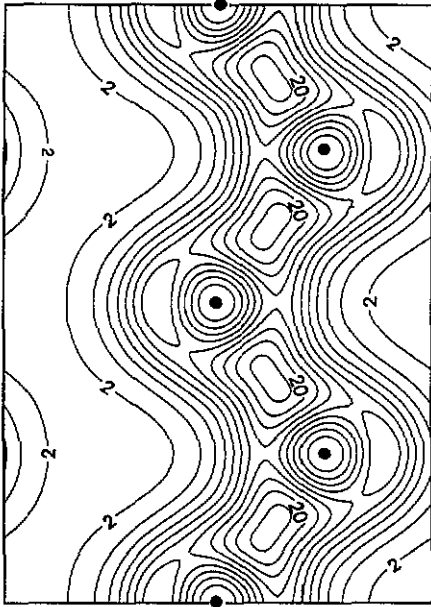
Figure 1. The electronic charge density in the [$\bar{1}10$] plane for the equilibrium lattice in germanium. This shows clearly the bond charges situated halfway between the ions whose positions are shown by a dot. The contours are in units of electrons per unit cell volume.
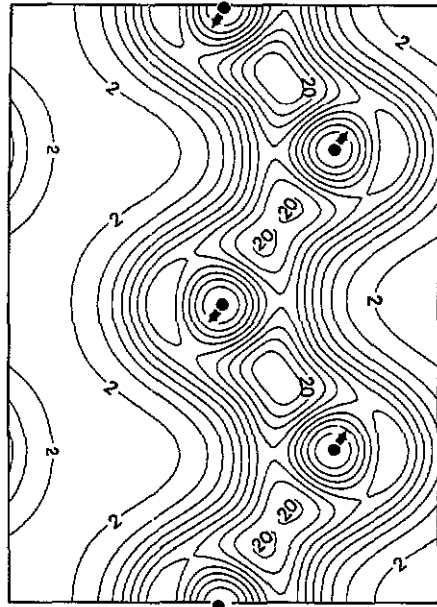
Figure 2. The electronic charge density for the germanium crystal when it is distorted by a LTO(Γ) phonon with $\delta R = 0.005$.

however, to ensure their exact agreement. This was done by an averaging process. For example, with $g = (2\pi/a)(5,3,1)$, we got two equations for $(\rho_N - \rho_R) + d_x$ from the TEC results and averaged them, two equations for $(\rho_N - \rho_R) + d_y$ and averaged these, and then two equations for $(\rho_N - \rho_R) + d_z$ and averaged these. The resulting three equations were then used as a basis for calculating $\rho_N - \rho_R, d_x, d_y$ and d_z. The fourth equation used is the orthogonality condition

$$g \cdot d(g) = 0. \tag{17}$$

This procedure obviously gives us a better measure of the first-order terms than can be achieved using the procedure of section 4 alone, because it uses all the calculated information. Also, if the charge densities were deduced using only the method of section 4, they would be inconsistent.

It is also interesting to note that if the pseudoatom is assumed rigid, there is only one variable in the linear equations and the values of $\sigma_1(g)$ connected by symmetry must satisfy several conditions.

We note that the relative size of any discrepancy of the TEC values from the required linear dependence is a measure of the importance of third- and higher odd-order anharmonic effects.
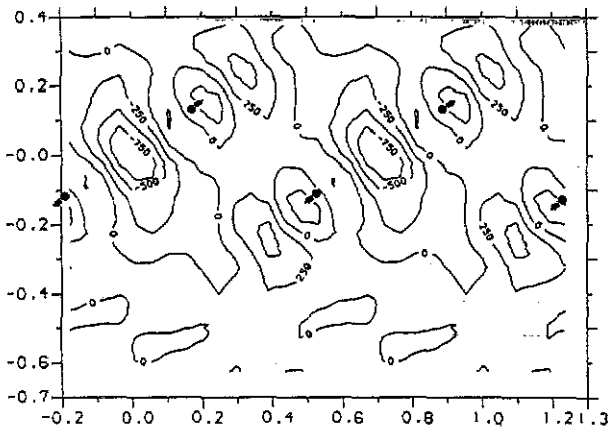
6. The results

In table 2 are presented the calculated values of the pseudoatom quantities ρ and d for the ion at R_s.
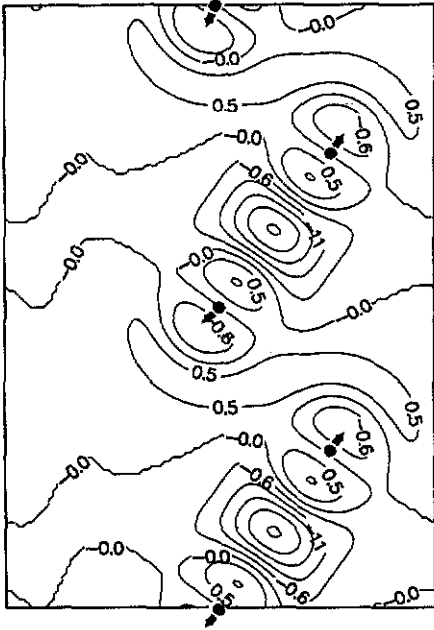
Figure 3. The change in electronic density due to the LTO(Γ) phonon with $\delta R = 0.005$ (i.e. figure 2 minus figure 1). It contains the harmonic and the anharmonic contributions.

Figure 4. As for figure 3 but due to the electronic rigid ion only. The units are in 10^{-3} electrons per unit cell.

Let us first look at the results for ρ. These calculations give both the real and the imaginary parts, which could not be achieved by using the perfect crystal TEC alone. It is also interesting to see that ρ_R at $g = (2\pi/a)(0,0,2)$ cannot be obtained from the perfect crystal. We note that ρ_R behaves fairly smoothly with g except possibly at $(3,3,1)$; there seems to be a sinusoidal variation, each oscillation decreasing by a factor of about 10. It is also noticeable that ρ_N is small in general and, for large g, is a factor of 10 smaller than ρ_R. These observations suggest that $\rho(r)$ does not deviate from spherical symmetry by large amounts. This suggests that a parametric model of the rigid ion could be fitted to these results (Ball 1990). Such a model might furnish information about the size and
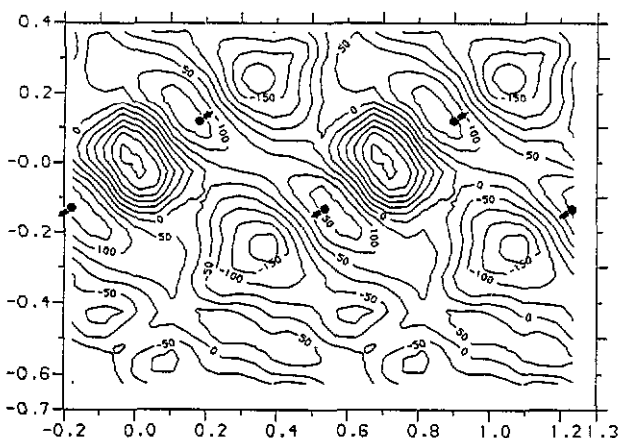
Figure 5. As for figure 4 but due to the deformation cnly.

shape of the rigid ion. The contour plots discussed below give some hint as to the shape of the rigid ion.

In comparing magnitudes of d and ρ, it should be remembered that the correct comparison is between d and $g\rho(g)$. It can be seen that the deformation is significant for the RLVs $(0,2,2)$ and $(1,1,3)$. It decreases at approximately the same rate as $g\rho$ for larger g. These results show that the deformation is a significant part of the pseudoatom and cannot be ignored. As rigid-ion models do not take deformation into account, our results show that such models at least lack physical suitability for the calculation of phonon frequencies in germanium. We believe that this is the first time that pseudoatom deformation has been explicitly shown to be present in significant amounts in a crystal.

To get some picture of the pseudoatom, we have drawn contour plots, in the plane with axes [110] and [001], of various contributions to the electron density. Figures 1–3 are obtained from the TEC and use 2277 RLVs. In figure 1 is drawn the electron density of the perfect crystal. In figure 2 is drawn the charge density when the two basis ions in the primitive unit cell have moved apart, i.e. $\delta R = 0.005$. Figure 3 shows the change in charge density between figures 1 and 2. This includes the anharmonic effects. In figures 4–6 the changes due to the electronic rigid ion, the deformation and to the complete electronic pseudoatom respectively are drawn. Figures 7–9 show the changes due to the anharmonic effects. Figures 4–9 were plotted using only the 416 RLVs of table 2. Because the effects of the pseudoatom decrease rapidly with g, no significant features in the contour plots are likely to be lost by using this smaller number of RVLs. This is also true for the anharmonic effects.

Figure 1 shows clearly the charges around the ions and the bond charges midway between the ions. Figure 2 shows that the stretching of the bond length results in a readjustment of the bond charge: the single broad maximum of the charge density in the perfect crystal has been deformed and now two maxima of equal magnitude appear which are symmetrically situated along the bonding direction. This arises because on bond-length stretching some charge is pushed away from the bond centre towards the region around the ions, as is clearly seen in the charge-difference plot, figure 3. (Exactly the opposite of this happens when compression of a bond length occurs.)

Figure 4 is consistent with a fairly spherically symmetric electronic rigid ion that has an atomic -type density, thereby increasing the density in the direction of the movement
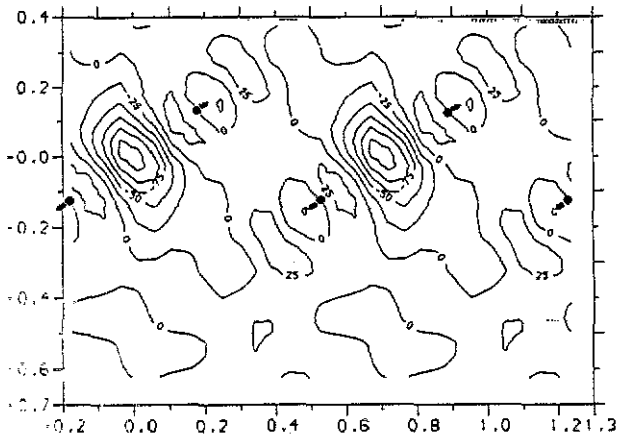
Figure 6. As for figure 4 but due to the complete electronic pseudoatom (i.e. the sum of figures 4 and 5). The units are in 10^{-2} electrons per unit cell.

of the neighbouring ion and decreasing it between the ions. This would give a dipolar effect at the ion, which is nullified by the core charge as the pseudoatom, with the core included, is in total neutral in charge. It looks as if there is very little contribution to the rigid ion from the bond charge.

The total change in charge density due to the deformation is zero, so that we can view the effect of the deformation as a transfer of charge. According to figure 5, the main effects of deformation seem to be a reduction in the bond charge by transferring the charge to the ion in such a way that the dipolar effect due to the electronic rigid ion is reduced. This is also confirmed by figure 6, and confirms our analysis of figures 1–3.

Our plot (figure 6) of the total first-order change is very similar to that of Resta (1983), although he used a dielectric matrix and fewer RLVs.

It should be remembered that the change in charge density due to the effect of pseudoatoms is linear in ionic movement. Thus, when this movement causes compression, i.e. $\delta R = -0.005$, the contour plots are the same but with the signs reversed. Similarly, when $\delta R = 0.015$, the contours are the same but the associated magnitudes are multiplied by three.

Figures 7–9 show the anharmonic change in the electronic charge density for $\delta R = 0.005, 0.015$ and -0.015 respectively. The changes (figure 7) for $\delta R = 0.005$ are small and show a slight increase in the charge at the bond charges between the separating ions. This contrasts with figure 8 where the bond charge is decreasing. The anharmonic effects (figure 9) when the ions move towards each other are straightforward: the bond charges are increased by an amount which is about half the increase due to the pseudoatom movement. In this case the anharmonic effect enhances the linear effect of the pseudoatom deformation which is to increase the bond charge (see above).

7. Summary

We have carried out total-energy calculations on the undistorted lattice of germanium and on lattice with a LTO(Γ) distortion. We separated the harmonic and anharmonic
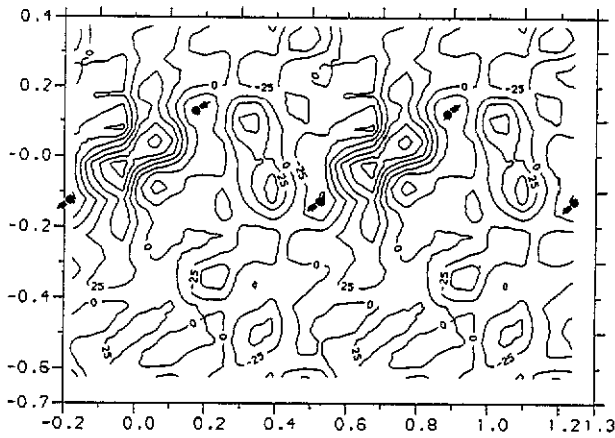
Figure 7. The change in the electronic density due to the anharmonic effects with $\delta RT = 0.005$. (This is like figure 3 minus figure 6 except that fewer RLVs are used). The units are in 10^{-3} electrons per unit cell.
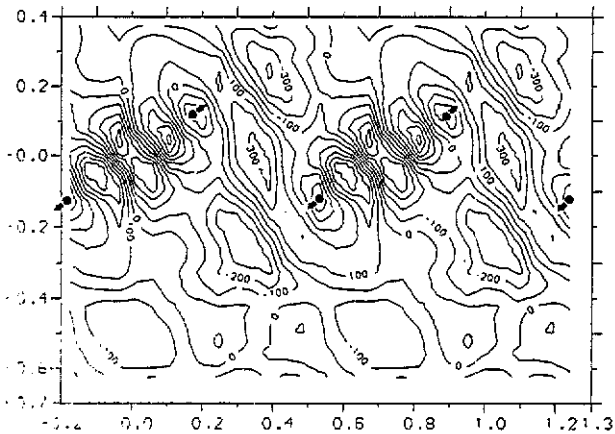
Figure 8. As for figure 7 but $\delta R = 0.015$.
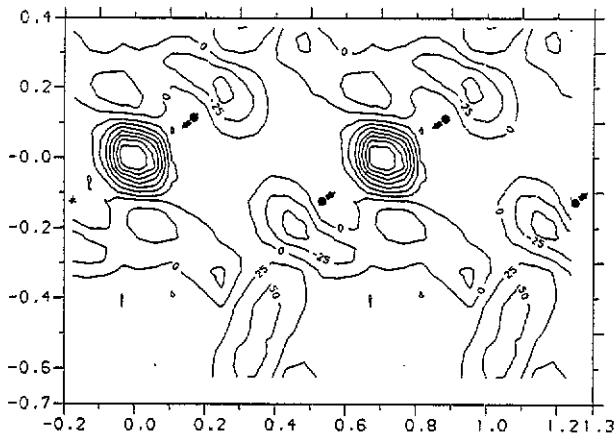
Figure 9. As for figure 7 but $\delta R = -0.015$.

parts of the changes in charge density and ensured that the former satisfied the symmetry requirements. We have used the results to calculate the Fourier components of the pseudoatom at reciprocal lattice vectors. We have found that the rigid ion behaves somewhat like an atom, and that the deformation is significant but smaller in magnitude and acts mainly at the bond charges. The total first-order change in the charge density due to a $LTO(\Gamma)$ phonon calculated in the present pseudoatom work is similar to the dielectric results of Resta (1983). The model of the pseudoatom constructed in this work can be developed further and applied to calculate phonon frequencies. We hope to investigate this in the future.

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