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UHF calculations of hyperfine coupling constants of anomalous muonium in C, Si and Ge

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Abstract. We have used the UHF-GTO cluster method to calculate the hyperfine coupling constants A_{\parallel} and A_{\perp} of anomalous muonium in C, Si and Ge according to the molecular radical model. Results for anomalous muonium in the bond-centred site are in good agreement with those obtained using the same method or semiempirical methods in larger clusters of C and Si. The new results for Ge successfully explain the sign and strength of A_{\parallel} , A_{\perp} and A_{\parallel}/A_{\perp} ; however the calculated contact and dipolar terms follow a monotonic behaviour in contrast with experimental results.

1. Introduction

When a positive muon is implanted in semiconductors, two different paramagnetic bound states, called normal muonium, Mu, and anomalous muonium, Mu*, give rise to a muon-spin–electron-spin hyperfine interaction, which can be observed in μ SR (muon spin rotation) experiments, whose aspects have been recently reviewed by Cox (1987) and Patterson (1988).

Different equilibrium sites where the muon ‘stops’ after thermalisation, together with the kind of defect that it introduces in the perfect crystal environment are believed to be responsible for these two different states. Theoretical investigations, which started at least fifteen years ago, seem currently to favour the molecular radical model proposed by Cox and Symons (1986).

In the Cox and Symons (CS) model the two muonium states are related to two different interstitial sites of a neutral muonium in the host semiconductor: the antibonding AB site for Mu and the bond-centred or BC-site for Mu*. A fast local tunnelling among four equivalent AB neighbours sites near the tetrahedral T site explains the observed isotropic hyperfine interaction of Mu. The axial symmetry of the Mu* coupling tensor along the $\langle 111 \rangle$ direction is instead explained assuming that the interstitial muon is at the centre of the X–X bond (X = C, Si, Ge in this paper) in diamond-type host crystals.

The hyperfine coupling tensor components are, in principle, defined except for their absolute sign, but, as a result of the observation of a Mu to Mu* transition in diamond (Odermatt *et al* 1986), it is possible to state that if the hyperfine constant A for normal muonium is positive then the isotropic component A_s , of the coupling tensor for anomalous muonium is negative and, consequently, the anisotropic component A_p is positive.

A large, positive and p-like spin density on two equivalent Si neighbours sites in the $\langle 111 \rangle$ direction has been determined from measurements of Si hyperfine structure of Mu^* in Si (Kiefl *et al* 1988); the features of the μSR spectral lines and the observed inversion symmetry of the Mu^* site are considered by those authors a proof of the BC model.

The Mu^* negative Fermi density at the muon site can also be explained by the vacancy-associated (VA) model in which a muon is trapped near a double-positively charged vacancy (V^{2+} site). Using the UHF approach in clusters $\text{X}_4\text{H}_{12}\text{Mu}$ of four host atoms surrounding the vacancy, Sahoo *et al* (1986) were able to obtain the direct trend of the Mu^* isotropic hyperfine constants, which is non-monotonic in going from C to Ge.

The non-monotonic behaviour of the Mu hyperfine constants in the group-IV semiconductors causes the cavity model (Wang and Kittel 1973) to fail because it predicts the wrong sequence in C, Si and Ge (Holzschuh *et al* 1982). Manninen and Meier (1982) have considered the influence of zero-point motion on the hyperfine constants in a model based on the density functional formalism in which the host lattice is described by a dielectric function and a pseudopotential accounting for the effective mass of the ground state of a hydrogenic deep donor. After zero-point motion, averaging their results again show the incorrect monotonic trend in the T as well as in the hexagonal H interstitial sites.

The effects of the lattice relaxation around the muon were considered for the first time by Mainwood and Stoneham (1984) together with zero-point motion influence in T and H sites of C and Si and in a detailed HF analysis of H in diamond by Estreicher *et al* (1986).

Relaxation effects are essential in order to confirm the validity of the CS model for Mu and Mu^* : it was shown from HF-PRDDO calculations in C and Si (Estle *et al* 1986, 1987) that a negative density and a minimum for the energy are achieved when the muon is placed in the centre of the bond whose length was increased by 42% in C and 35% in Si. A second minimum, with the muon at the T site and a small outward relaxation of the nearest-neighbours host atoms, is higher in energy than the BC site; the Mu to Mu^* transition is explained in terms of this interstitial metastability of the muon (or H) in C and Si.

MINDO/3 calculations (Deak *et al* 1988) give 34% relaxation at the BC site in Si; in this last paper normal Mu is found in the AB site displaced 0.4 Å from the T site in the $\langle 111 \rangle$ direction.

Using the local density functional formalism, the AB site (0.3 Å from T) was found to be more stable than the BC site (35% relaxed) in Si (Sasaky and Katayama-Yoshida 1988); the same approach gives the BC site (34% relaxed) as being more stable than the T site (Van der Walle *et al* 1988). UHF-GTO calculations on $\text{Si}_{10}\text{H}_{17}$, and Si_8H_{19} clusters (Amore *et al* 1988) give similar results: an absolute minimum in the BC site 35% relaxed and a second minimum in the T, while the AB site is not stable at all.

However, up to now, comparison with experimental data for the whole series C, Si and Ge could not be done both for Mu and Mu^* because results are available only for C and Si and none for Ge, except for the vacancy-associated model.

In this paper we shall confine our attention to the BC model. Our main purpose is to obtain results for C, Si and Ge to compare with experimental HF constant values in their sign, values and particularly in their trend. This was done using the same UHF method supposing that the muon introduces the same kind of defect, i.e. the relaxed bond-centred configuration, in clusters, attempting to simulate the real crystal environment in a balanced way for all the elements of the series.

Table 1. Experimental data and theoretical results of the BC model of anomalous muonium in diamond, silicon and germanium. Relaxation distances of two NN X atoms to the muon (X = C, Si, Ge) are in Å; the * marks the perfect crystal X–X bond length. A_s and A_p are the isotropic and anisotropic components of the hyperfine coupling tensor in MHz.

Host	A_s	A_p	X–X	Method	Reference
C	–205.7	186.9	1.54*	exp.	Patterson (1988)
Si	–67.4	25.3	2.35*	exp.	Patterson (1988)
Ge	–96.5	34.6	2.45*	exp.	Patterson (1988)
C	<0	>0		mol. radical	Cox and Symons (1986)
Si	<0	>0		mol. radical	Cox and Symons (1986)
Ge	<0	>0		mol. radical	Cox and Symons (1986)
C	–320		2.14	UHF-GTO	Claxton <i>et al</i> (1986)
C	–848	>0	2.2	PRDDO	Estle <i>et al</i> (1987)
Si	<0	>0	3.17	PRDDO	Estle <i>et al</i> (1987)
Si			3.15	MNDO	Deak <i>et al</i> (1988)
Si	small		3.19	LDA	Sasaki and Katayama-Yoshida (1988)
Si			3.15	LDA	Van de Walle <i>et al</i> (1988)
Si	–192		3.19	UHF-GTO	Amore <i>et al</i> (1988)

The first problem to consider is the choice of cluster size; the natural possibilities are (i) to include the nearest-neighbour X atoms around Mu, giving a cluster $X_2L_6\text{Mu}^*$, where L is a suitable ligand to saturate the dangling bonds of X atoms; (ii) to include second-nearest-neighbours, giving $X_8L_{18}\text{Mu}^*$; (iii) to include third-nearest-neighbours, i.e. $X_{26}L_{54}\text{Mu}^*$, and so on.

Owing to the computational limits of our code, we cannot perform calculations in clusters larger than $X_2L_6\text{Mu}^*$ with Ge atoms. Therefore we have chosen this small cluster (sc) model where the muon is placed in the middle of the X–X bond.

A second problem is the proper choice of the saturating ligand L. The most common choice so far has been hydrogen. However in such a case the dangling bonds are polarised in a different way from atom to atom and this might introduce spurious effects on the final results. This point is obviously expected to be important with small clusters and when the trend along the series is studied. Therefore we also adopted as ligands pseudo-atoms chosen in such a way as to ensure non-polar bonds.

As will be shown that the sc model, despite its smallness, basically gives results in agreement with those already obtained in larger clusters of C and Si. New results for Ge successfully explain the sign and strength of A_{\parallel}/A_{\perp} , A_s , A_p ; however the non-monotonic trend is not obtained in our calculations.

2. Results and discussion

Experimental, as well as previous theoretical, data are reported in table 1. Our results are reported in tables 2 and 3, where experimental values are repeated for ease of comparison.

Our computations were all performed by *ab-initio* LCAO-UHF method using the standard STO-3G gaussian bases for C and Si and a minimal basis of comparable quality for Ge (Huzinaga *et al* 1984). The hyperfine coupling constants were calculated from the *ab-initio* wavefunctions after annihilation of the spin-quartet component using well

Table 2. Results for clusters $X_2(L)_6\text{Mu}^*$ of D_{3d} symmetry, Mu in the bc site; X = C, Si, Ge; L, ligand, pseudo-atom or CH_3 ; R_1 , distance X-Mu*; R_2 , distance X-L, in Å; α , angle L-C-Mu*, in degrees; Z, charge of pseudo-atom in au (except in case of CH_3 ligand); A_s , A_p , isotropic and anisotropic components of hyperfine coupling tensor at the Mu, in MHz; $C(Y)$, Mulliken electron population on centre Y in au ($Y = \text{Mu}^*$, X, L); the * marks the Z value which equalises the Mulliken charges in the $C_2(L)_6$ pseudo-molecule.

Host	R_1	R_2	α	Z	A_s	A_p	C(Mu)	C(C)	C(L)	Ligand
C	1.155	1.494	96.89	4.00	-287	272	0.90	5.69	1.12	pseudo
				3.63*	-293	269	0.92	5.96	1.03	pseudo
				1.00	-272	275	1.06	7.58	0.46	pseudo
				=	-306	262	0.89	6.03	6.03	CH_3
Si	1.557	2.251	101.21	4.00	-226	104	1.11	12.36	1.53	pseudo
				1.61*	-254	122	1.17	13.96	0.98	pseudo
				1.00	-260	122	1.18	13.64	0.85	pseudo
Ge	1.600	2.406	101.49	4.00	-174	71	1.08	31.49	1.16	pseudo
				3.29*	-186	76	1.05	31.87	1.04	pseudo
				1.00	-201	80	0.95	33.34	0.56	pseudo

known relations (Sahoo *et al* 1986). In order to account for the poor behaviour of the gaussian orbitals near the nuclei, the resulting Fermi terms were normalised to the corresponding STO-3G hydrogen atom value 0.395.

Our computations can be classified according to the type of saturation adopted for the dangling bonds and the cluster geometry chosen. In $X_2\text{H}_6$ molecules, the Mulliken population analysis shows a non-negligible bond polarity and a remarkably different behaviour of the three host atoms. At equilibrium bond lengths, C and Ge atoms are negatively charged, while Si atoms are positive. In ethane the bond polarity can be eliminated by stretching the C-H distance; when C-H is 1.541 Å, the Mulliken charge on carbon is approximately zero. This distance happens to be also the equilibrium C-C value in diamond and sigma bonds. When this value of C-H is adopted in clusters $C_{10}\text{H}_{16}\text{Mu}$ (*adamantane*), the value of the Fermi interaction for normal muonium in the T site turns out as expected to be less than its vacuum value. This suggests that bond polarity is of special importance in this kind of calculation.

On the other hand, if one performs a UHF calculation on the radical molecule $C_{10}\text{H}_{16}\text{Mu}$ the total spin $\langle S^2 \rangle$ deviates considerably from the theoretical value for a doublet, 0.75. This is rather unpleasant if one wants to compute a spin-dependent property, even if the main spin contamination is probably localised on the outer C-H bonds rather than on the muon site.

As far as silicon is concerned, it seems there is no way to balance the Mulliken charges by changing the Si-H distance; when Si-H is taken equal to equilibrium Si-Si, we are far from balance, and a residual non-negligible positive charge is still found at Si-H distances as long as 5 au.

In case of germanium, balance would be achieved by compressing the Ge-H bond instead of stretching it. Thus, from this point of view, there is no way to treat the three elements C, Si and Ge on an equal footing. For this reason we resort to the use of pseudo-atoms as saturators of the dangling bonds. These pseudo-atoms are intended to simulate the real atoms of C, Si or Ge to which the dangling bonds are connected. The idea has been developed by several authors (Laszlo 1982 and references therein) and is known to be a better alternative to hydrogen atoms in many cases; Mainwood and Stoneham

(1983) have also used pseudo-atoms to study interstitial muons and hydrogen in large Si clusters. We choose our saturators to comprise a point charge of value Z supporting a single sp^3 hybrid orbital pointing to the atom to be saturated. The sp^3 hybrid is built with the outer s and p atomic valence orbitals of the given atom. The choice of Z poses problems requiring some consideration. In a perfectly neutral lattice each atom has a nuclear charge equal to the number of its electrons, and therefore a value of $Z = 1$ should be appropriate for our saturators. However, the Mulliken charges turn out to be badly unbalanced in this case. A value $Z = 4$ is suggested by consideration of the screening of the nuclear charge by the inner electrons, but, again, we do not get neutrality. We chose to treat Z as an adjustable parameter and explored the range $Z = 1$ to $Z = 4$. A fractional value of Z in this interval could be interpreted as an effective nuclear charge accounting for the screening of the valence electrons missing on the pseudo-atom. We determined the value of Z by performing calculations on $X_2(\text{sat})_6$ pseudo-molecules where all angles and bond lengths are taken to be equal to those in the perfect crystal lattice we want to simulate.

Within some hundredths of atomic units, we have found the charge neutrality achieved at values of Z equal to 3.63, 1.61, 3.29 respectively for C, Si and Ge. The value for silicon is much smaller than the other two, according to its behaviour in Si_2H_6 .

In table 2 we report the values of hyperfine parameters computed at this value of Z , together with the two extreme cases $Z = 1$ and $Z = 4$. The influence of the Z variation on the HF constants is small, not enough to alter significantly their trend and values; these values also compare favourably with the results of the C_8H_{19} cluster (tetra-methyl-butane + muon) where each pseudo-atom is replaced by a CH_3 group.

As far as geometry relaxation is concerned, we adopted two different criteria. In the first, hereafter referred to as case (A), the geometry is optimised using the MNDO (Dewar 1977) method. We started from a cluster $(\text{XH}_3)_3\text{X}-\text{X}(\text{XH}_3)_3$ where $\text{X} = \text{C}, \text{Si}, \text{Ge}$ of D_{3d} symmetry with bond lengths and angles taken from the equilibrium geometry of the X_8H_{18} molecules. The H atoms were then kept fixed in space, a muon was placed at the centre of the inner $\text{X}-\text{X}$ bond. The positions of the eight X atoms were then optimised with the constraint of D_{3d} symmetry.

The resulting first-neighbour relaxations compared with all known results in table 1 are slightly larger for C and shorter for Si. By denoting the second NN X atom with X' , $\text{Mu}-\text{X}-\text{X}'$ angles are 97.9° , 101.2° , 101.5° and $\text{X}-\text{X}'$ distances 1.494 Å, 2.251 Å, 2.406 Å. Second NN in C are found in the same positions obtained in larger $\text{C}_{44}\text{H}_{42}\text{Mu}^*$ clusters (Estle *et al* 1987), where relaxation up to second NN was included in *ab-initio* calculations.

We repeated the computations using the same geometry but replacing the pseudo-atoms with hydrogens at a number of $\text{X}-\text{H}$ distances. The results are not reported for sake of simplicity, but do not show any significant difference from those in table 2. Therefore, bond polarity in itself does not seem to be essential in this context.

In order to have a better insight into the basic features involved in understanding the BC model, we have also adopted a second, more qualitative model of the cluster used for the computation of the HF constants. Consider two XL_3 fragments connected by a bond $\text{X}-\text{X}$ of given length $R(\text{X}-\text{X})$ and let the muon move along the bond itself. The resulting potential energy profile changes its nature as a function of $R(\text{X}-\text{X})$: when $R(\text{X}-\text{X})$ is less than a critical value R^* , about twice the $\text{X}-\text{H}$ bond length, the profile has a single minimum in the centre. This minimum is a sharply decreasing function of $R(\text{X}-\text{X})$ until R^* is reached. For $R(\text{X}-\text{X})$ greater than R^* , we have a double-minimum profile and the total energy of the cluster is approximately constant: the cluster is now dissociated in XH_3Mu and XH_3^+ . We consider the real potential energy of the crystal to be the sum

Table 3. Summary of computed and experimental hyperfine constants (MHz) of anomalous muonium in C, Si and Ge.

Host	A_s	A_p	A_{\parallel}	A_{\perp}	A_{\parallel}/A_{\perp}
(1) Experiment:					
C	-205.70	186.9	168.1	-392.6	-0.43
Si	-67.30	25.3	-16.7	-92.6	0.18
Ge	-96.50	34.6	-27.3	-131.1	0.21
(2) v_A model (Sahoo <i>et al</i> 1986):					
C	-85.0	69.5	54.0	-154.5	-0.35
Si	-55.0	16.0	-23.0	-71.0	0.32
Ge	-70.0	12.5	-45.0	-82.5	0.55
(a) BC model (this work), pseudo-atoms as ligands, optimised:					
C	-292.8	269.2	245.6	-562.0	-0.44
Si	-254.0	122.4	-9.2	-376.4	0.02
Ge	-185.6	76.1	-33.4	-261.7	0.13
(b) BC model (this work), hydrogens as ligands, not optimised:					
C	-273.0	223.0	173.0	-496.0	-0.35
Si	-235.0	103.0	-29.0	-338.0	0.09
Ge	-194.0	65.0	-64.0	-259.0	0.25
(c) BC model (this work), zero-point motion average of (b):					
C	-231.0	178.0	125.0	-409.0	-0.31
Si	-201.0	82.0	-37.0	-283.0	0.13
Ge	-168.0	44.0	-80.0	-212.0	0.38

of the local X–Mu–X interaction given above and a lattice relaxation involving the other atoms, and adopt the value R^* as an estimate of the $R(X\text{--}Mu)$ distance in the relaxed crystal. This amounts to assuming that the lattice reaction to distortion is not strong enough to overcome the steep rise in the X–Mu–X local interaction for $R(X\text{--}X)$ less than R^* , but it is dominating in the region where the energy profile is flat, i.e. for $R(X\text{--}X) > R^*$. This choice of geometry is referred to as case (B), and it can be combined with either choice of ligands. Both hydrogens and pseudo-atoms have been employed with similar results and we report only the data for hydrogens. The X–H bond length was chosen equal to equilibrium bond length of the corresponding molecule (Estreicher *et al* 1985); this enables comparison with previous results obtained adopting this choice. In this way we have found the following relaxation distances for X–X bond: 2.38 for carbon, 3.05 for silicon and 3.24 Å for germanium, as shown in table 3. The results are essentially in agreement with our previous ones, and with calculations for larger clusters reported in table 1.

In this case (B) we also performed a zero-point motion average of the computed values of hyperfine parameters in order to evaluate its importance. This implies the computation of the potential energy surface when the muon is moved outside the X–X bond. A summary of our results is reported in table 3, where experimental data and values from the vacancy model are also displayed. In this table we also show the values of the hyperfine tensor components A_{\parallel} and A_{\perp} , which are nothing but a linear combination of A_s and A_p (e.g. see table 1 of Cox 1987); however they compare better with experiment, at least in the behaviour of the A_{\parallel} component, which now has the expected trend.

Although we have not included long-range relaxation, we estimate the correction to be approximately 10 MHz for one per cent variation of the X–X distance for A_s and less for A_p in the three hosts; in other words we do not expect this correction to modify the monotonic trend. The same conclusions can be outlined even if zero-point motion is taken into account: zero-point motion corrections can be expressed in terms of nearly equal percent lowering of the HF constants, their trend is not modified by such treatment. This was done in case (B), after computation of the potential energy surface when the muon is moved outside the X–X bond; the resulting mean values of the HF constants averaged, in a variational treatment, over the ground state of the corresponding spatial anharmonic oscillator are shown in table 3.

The agreement with larger cluster calculations was more evident when, surprisingly, we found a cavity effect (Claxton *et al* 1986) without cavities. In case (B), if the muon is moved in the direction perpendicular to the bond towards the vacuum, the A_s constant becomes positive and greater than the vacuum value at a distance approximately equal to that of the τ site from the BC site in *adamantane*. This happens because at large distances from the BC site the HOMO (highest occupied molecular orbital) of the X_2H_6Mu system is an atomic-like $1s$ orbital centred on muon, and this provides a spin density essentially equal to that of the isolated muonium atom. At the same time, the Mu $1s$ orbital participates to a very small extent in some deep lying bonding molecular orbitals of g symmetry. If the muon is moved close to the bond the HOMO–LUMO (lowest unoccupied molecular orbital) energy gap decreases reaching a crossing point obviously associated with configurational instabilities. A new configuration is now stabilised where the Mu $1s$ is now contributing to the LUMO of the system and to bonding orbitals of g symmetry with valence orbitals of neighbour atoms. Configuration interaction or multi-configuration-SCF methods should therefore be employed to compute wavefunctions and total energies in the crossing region.

3. Conclusions

We have calculated the HF components of anomalous muonium Mu^* in the bond-centred BC-site giving for the first time results for the whole series C, Si and Ge, which enables full comparison with experimental data. Some of the observed features are explained: negative A_{\perp} and opposite signs of A_{\parallel} and A_{\perp} in C, the same sign of A_{\parallel} and A_{\perp} in Si and Ge, the right non-monotonic behaviour of A_{\perp} and of A_{\parallel}/A_{\perp} (table 3). Moreover the SC model basically reproduces the HF components values obtained using larger clusters corresponding with a given relaxed geometry and saturator bond length.

Nevertheless the SC model of Mu^* in the BC site at this level of approximation predicts a monotonic behaviour both for the Fermi and dipolar hyperfine constants in contrast with the non-monotonic experimental data.

The VA model, at a similar level of approximation ($STO-3G$ and $X_4H_{10}Mu^*$) gives, at least for the Fermi terms, the expected trend and all the observed features as examined from the point of view of the tensor components A_{\parallel} and A_{\perp} .

However, before drawing final conclusions, one should be aware of many inherent limitations of the present calculations. Minimal basis set ($STO-3G$) and cluster smallness can be responsible, among other reasons, for the lack of results.

On the other hand, Das has discussed the viability of a model which combines the features of the VA and BC models (Das 1988).

We cannot conclude that the BC model is wrong, owing to the problems in cluster calculations described above not being completely resolved as yet; we have shown that the BC model also successfully explains the HF constants in germanium alone. This fact suggests that, independent of the method used, a single-host theoretical approach is not very useful for a complete understanding of the Mu^* problem.

More careful investigations are required and, in our opinion, more reliable results can be obtained if the same method is used in calculations for the three group-IV semiconductors C, Si and Ge with the aim of reproducing the correct behaviour of the hyperfine constants for Mu as well as for Mu^* . Further confirmation of the CS model can be given by the calculations in GaP and GaAs, which we are going to do using the same CS model of Mu^* described in this paper.

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