LANDOLT-BÖRNSTEIN

Numerical Data and Functional Relationships in Science and Technology

New Series
Editor in Chief: O. Madelung

Group III: Crystal and Solid State Physics

Volume 22
Semiconductors

Supplements and Extensions to Volume III/17

Editors: O. Madelung · M. Schulz

Subvolume b

Impurities and Defects in Group IV Elements and III-V Compounds

C. A. J. Ammerlaan · W. Bergholz · B. Clerjaud · H. Ennen · H. G. Grimmeiss
B. Hamilton · U. Kaufmann · W. v. Münch · R. Murray · R. C. Newman
A. R. Peaker · G. Pensl · H.-J. Rath · R. Sauer · J. Schneider · M. Schulz
M. S. Skolnick · N. A. Stolwijk · P. Vogl · A. F. W. Willoughby · W. Zulehner

Edited by M. Schulz

Springer-Verlag Berlin Heidelberg New York
London Paris Tokyo Hong Kong

4.1.3 Paramagnetic centers

4.1.3.0 Introduction

Electron paramagnetic resonance (EPR) spectra are conveniently analyzed using a spin-Hamiltonian. In the concept of the spin-Hamiltonian, the energies of the levels comprising the ground state are expressed in terms of a polynomial in the effective electron spin operators $\boldsymbol{S}$ and, when magnetic nuclei are present, nuclear spin operators $\boldsymbol{I}$. A small number of constants in the spin-Hamiltonian $\mathscr{H}$ can accurately describe the observed transitions. A general form suitable to analyze and identify the spectra observed in diamond is: $\mathscr{H} = \sum \mathscr{H}_i$.

In the spin-Hamiltonian required to analyze the spectroscopic data, the following terms may appear:

Zeeman effect

$$\mathscr{H}_1 = \mu_B \boldsymbol{B} \cdot \mathbf{g} \cdot \boldsymbol{S}$$

$\mathscr{H}_1$ describes the electronic Zeeman effect. All paramagnetic centers have this interaction. Due to the small value of the spin-orbit coupling constant in diamond and the strong crystal field in the solid which effectively quenches orbital contributions to the magnetic moment, the g-values for nearly all centers are close to the free-electron value $g = 2.0023$. Identification of spectra on the basis of the **g**-tensor only, the common situation for centers in silicon, is not possible in diamond. Other spin-Hamiltonian constants or characteristics of the spectrum have to be used additionally.

Zero-field splitting

$$\mathscr{H}_2 = \boldsymbol{S} \cdot \mathbf{D} \cdot \boldsymbol{S}$$

$\mathscr{H}_2$ represents the zero-(magnetic)-field splitting. The interaction is only present for electron spin $S \geq 1$. The identification of centers produced by irradiation, notably the R-spectra, mainly rests on the symmetry and components of the **D**-tensor.

Higher-order Zeeman effect

$$\mathscr{H}_3 = g_2 \mu_B (B_x S_x^3 + B_y S_y^3 + B_z S_z^3)$$

$\mathscr{H}_3$ represents the rather rare higher-order Zeeman effect which can be present in case $S \geq 3/2$, and has the given form for centers of cubic symmetry. The interaction in diamond has been reported for one center only, i.e. the acceptor-related spectrum NL1.

Normal-strain effect

$$\mathscr{H}_4 = b(\varepsilon_{xx} S_x^2 + \varepsilon_{yy} S_y^2 + \varepsilon_{zz} S_z^2)$$

$\mathscr{H}_4$ expresses the effect of normal strains of the diamond crystal on the spectrum in terms of the deformation potential constant b and normal components of the strain tensor ε_{xx}, ε_{yy} and ε_{zz}. This term was only reported for the analysis of acceptor-related spectrum NL1.

Shear-strain effect

$$\mathscr{H}_5 = (d\sqrt{3}/3)[\varepsilon_{xy}(S_x S_y + S_y S_x) + \varepsilon_{yz}(S_y S_z + S_z S_y) + \varepsilon_{zx}(S_z S_x + S_x S_z)]$$

$\mathscr{H}_5$ expresses, similar to the previous term, the effect of distortion of the crystal on the energy levels. The deformation potential constant is d, the components of the shear strain are ε_{xy}, ε_{yz} and ε_{zx}. This term was only reported for spectrum NL1.

Nuclear Zeeman effect

$$\mathscr{H}_6 = -g_n \mu_N \boldsymbol{B} \cdot \boldsymbol{I}$$

$\mathscr{H}_6$ gives the Zeeman interaction energy for a nucleus with spin I. The nuclear Zeeman splitting is not observable in first order in EPR. It can be measured by electron-nuclear double resonance (ENDOR) and then leads to unambiguous identification of an impurity through the nuclear magnetic moment (g_n). Only a few studies by ENDOR have been performed for centers in diamond; examples include P1 [66C] and P2 [73L3, 84W].

Hyperfine interaction

$$\mathscr{H}_7 = \boldsymbol{S} \cdot \mathbf{A} \cdot \boldsymbol{I}$$

$\mathscr{H}_7$ describes the hyperfine interaction between the electron(s) in the paramagnetic defect and a nucleus with spin I. The term has to be summed over all the nuclei with non-zero spin for which an interaction is resolved. For spectra in diamond always the isotope ^{13}C, with nuclear spin $I = 1/2$, has to be considered. Due to the low abundance 1.1% of this isotope, the structural details in spectra related to this nuclear

interaction have a relatively low intensity. Nitrogen, with $I=1$ of the 99.63% abundant isotope ^{14}N, is the most common impurity in diamond. The hyperfine splitting into three sets of components reveals the presence of one or several nitrogen atoms. The identification of spectra given in Table 1 is based on this characteristic hyperfine structure. Actual observations have been made for carbon, nitrogen and a few other magnetic impurity isotopes. The hyperfine interaction can give characteristic structure to the EPR spectra, valuable for identification and further understanding of the atomic and electronic structure of the centers.

Nuclear quadrupole interaction

$$\mathcal{H}_8 = I \cdot \mathbf{Q} \cdot I$$

$\mathcal{H}_8$ represents the nuclear quadrupole effect. Only effective when $I \geq 1$, for example for ^{14}N, but not for ^{13}C. Being a purely nuclear interaction it is difficult to observe in EPR [65L]. ENDOR allows a more accurate determination of the quadrupole tensor, for instance for spectrum P1 [66C].

Nuclear exchange energy

$$\mathcal{H}_9 = J I_i \cdot I_j$$

$\mathcal{H}_9$ expresses the exchange interaction between nuclei and is effective when more than one impurity with nuclear spin is present in the center, such as in nitrogen aggregates. A measurement exists for the P2 center [73L3].

For further information on EPR see section 3.3. The convention adopted for silicon has been followed to label the spectra. Labels already in use in the literature were copied. Spectra which so far were not labeled, have been given designations. The new labels are: A9, A10, A11, E1, G1, KY1, L1, N5, N6, N7, O2, and TI1.

4.1.3.1 Nitrogen-related centers

Properties of EPR spectra related to nitrogen in diamond are compiled in Table 1.

Table 1. EPR spectra of nitrogen-related centers.

Spectrum N1 (Fig. 3)	
Symmetry:	monoclinic-I
Spin:	$S=1/2$
g-tensor:	$(g_1+g_2+g_3)/3=2.0024$
A-tensor:	nucleus ^{14}N, spin $I=1$, abundance 99.63%, 1 site $A_\parallel=130.0$ MHz, $\parallel$ [1, 1, 1] $A_\perp=$ 89.7 MHz, $\perp$ [1, 1, 1], [69S] 90.2 MHz, $\perp$ [1, 1, 1], [85L2]
A-tensor:	nucleus ^{14}N, 1 site $A_\parallel=9.0$ MHz, $\parallel$ [1, 1, 1], [69S] $A_\perp=8.1$ MHz, $\perp$ [1, 1, 1] $A_\parallel=8.3$ MHz, $\parallel$ [1, 1, 0], [85L2] $A_\perp=7.9$ MHz, $\perp$ [1, 1, 0]
A-tensor:	nucleus ^{13}C, spin $I=1/2$, abundance 1.1%, 3 sites $A_\parallel=33.6$ MHz $A_\perp=25.8$ MHz
A-tensor:	nucleus ^{13}C, 3 sites $A_\parallel=22.5$ MHz $A_\perp=20.7$ MHz
A-tensor:	nucleus ^{13}C, 2 sites $A_\parallel=18.9$ MHz $A_\perp=15.6$ MHz
Diamond:	natural type Ia and Ib
Model:	ionized nitrogen pair, negative (vacancy+nitrogen pair) complex, non-planar N_1CCN_2-complex, see Fig. 3
Reference:	69S, 72S, 78S, 82L1, 85L2

Spectrum N3

Symmetry: low
Spin: $S=1/2$
g-tensor: $g_1=2.0024$, $\parallel$ [1, 1, 1]
$g_2=2.0024^5$, $\perp$ [1, 1, 1]
$g_3=2.0024^5$, $\perp$ [1, 1, 1]
A-tensor: $A_\parallel=5.1$ MHz, axis 6° off [1, 1, 1]
$A_\perp=1.5$ MHz
Diamond: natural type I
Model: (nitrogen + divacancy) complex
Reference: 72S

Spectrum N4

Symmetry: trigonal
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.0025$
A-tensor: nucleus ^{14}N, spin $I=1/2$, abundance 99.63%, 1 site
$A_\parallel=91.4$ MHz, $\parallel$ [1, 1, 1]
$A_\perp=66.7$ MHz, $\perp$ [1, 1, 1]
A-tensor: nucleus ^{14}N, 1 site
$A_\parallel=89.7$ MHz, $\parallel$ [1, 1, 1]
$A_\perp=65.0$ MHz, $\perp$ [1, 1, 1]
Diamond: natural, brown, plastically deformed
Remark: anisotropic distribution of orientations
Model: substitutional nitrogen pair near dislocation
Reference: 75S, 78W

Spectrum OK1

Symmetry: monoclinic-I
Spin: $S=1/2$
g-tensor: $g_1=2.0031$, $\parallel$ [0 , −0.7071, +0.7071]
$g_2=2.0019$, $\parallel$ [+0.7096, +0.4983, +0.4983]
$g_3=2.0025$, $\parallel$ [−0.7046, +0.5017, +0.5017]
A-tensor: nucleus ^{14}N, spin $I=1$, abundance 99.63%
$A_1=15.48$ MHz, $\parallel$ [0 , −0.7071, +0.7071]
$A_2=21.66$ MHz, $\parallel$ [+0.4266, −0.6409, −0.6409]
$A_3=15.19$ MHz, $\parallel$ [+0.9063, +0.2988, +0.2988]
Q-tensor: nucleus ^{14}N
$Q_1=+1.31$ MHz, $\parallel$ [0 , −0.7071, +0.7071]
$Q_2=-2.67$ MHz, $\parallel$ [+0.5892, −0.5713, −0.5713]
$Q_3=+1.36$ MHz, $\parallel$ [+0.8080, +0.4166, +0.4166]
A-tensor: nucleus ^{13}C, spin $I=1/2$, abundance 1.1%, 2 sites
$A_{xx}=23.7$ MHz, $\parallel$ [1, 0, 0]
A-tensor: nucleus ^{13}C, 2 sites
$A_\parallel=13.5$ MHz
$A_\perp=9.9$ MHz
Diamond: natural type Ib
Model: (nitrogen + vacancy) complex, (nitrogen + vacancy + oxygen) complex
Reference: 70K, 72S, 77M, 78S, 88B

Spectrum P1 (Figs. 1, 4 and 12)

Symmetry: trigonal (crystallographic pointgroup 3m)
Spin: $S=1/2$

g-tensor: $g_{\parallel} = +2.0024$, $\parallel$ [1, 1, 1]
$g_{\perp} = +2.0024$, $\perp$ [1, 1, 1]

A-tensor: nucleus ^{14}N, spin $I=1$, abundance 99.63%, 1 site
$A_{\parallel} = 114.034$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp} = 81.325$ MHz, $\perp$ [1, 1, 1]

Q-tensor: nucleus ^{14}N, 1 site
$Q_{\parallel} = -2.649$ MHz, $\parallel$ [1, 1, 1]
$Q_{\perp} = +1.325$ MHz, $\perp$ [1, 1, 1]

A-tensor: nucleus ^{15}N, spin $I=1/2$, abundance >90%, 1 site
$A_{\parallel} = 163$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp} = 117$ MHz, $\perp$ [1, 1, 1]

A-tensor: nucleus ^{13}C, spin $I=1/2$, abundance 1.1%, 1 site
$A_{\parallel} = 340.8$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp} = 141.8$ MHz, $\perp$ [1, 1, 1]

A-tensor: nucleus ^{13}C, 3 sites
$A_{\parallel} = 41.03$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp} = 32.06$ MHz, $\perp$ [1, 1, 1]

A-tensor: nucleus ^{13}C, 3 sites
$A_{\parallel} = 23.3$ MHz, $\parallel$ [1, $\bar{1}$, $\bar{1}$]
$A_{\perp} = 26.8$ MHz, $\perp$ [1, $\bar{1}$, $\bar{1}$]

A-tensor: nucleus ^{13}C, 3 sites
$A_{\parallel} = 14.5$ MHz, $\parallel$ [1, $\bar{1}$, $\bar{1}$]
$A_{\perp} = 11.2$ MHz, $\perp$ [1, $\bar{1}$, $\bar{1}$]

A-tensor: nucleus ^{13}C, 6 sites
$(A_1 + A_2 + A_3)/3 = 8.24$ MHz

A-tensor: nucleus ^{13}C, 3 sites
$(A_1 + A_2 + A_3)/3 = 4.15$ MHz

A-tensor: nucleus ^{13}C, 6 (or 9) sites
$(A_1 + A_2 + A_3)/3 = 2.75$ MHz

Diamond: synthetic and natural type Ib, type Ia [81B, 82F1]

Remarks: anisotropy in **g**-tensor not measurable
hyperfine tensor **A**(^{14}N) and quadrupole tensor **Q**(^{14}N) measured by ENDOR [66C]
A_{xy} temperature dependent: $A_{xy} = 10.903$ MHz at 4.2 K, $A_{xy} = 10.880$ MHz at 300 K
hyperfine tensor **A**(^{15}N) measured in synthetic enriched ^{15}N doped diamond [75K]

Model: neutral substitutional nitrogen, $\langle 1,1,1 \rangle$ distorted, see Fig. 4

Reference: 59S1, 65D, 65L, 66C, 71S4, 74S, 75K, 78L2, 80A, 81A2, 81B, 82F1

Spectrum P2 (Figs. 2 and 5)

Symmetry: trigonal

Spin: $S=1/2$

g-tensor: $g_{\parallel} = 2.0025$, $\parallel$ [1, 1, 1]
$g_{\perp} = 2.0031$, $\perp$ [1, 1, 1]

A-tensor: nucleus ^{14}N, spin $I=1$, abundance 99.63%, 3 sites
$A_{\parallel} = 11.0$ MHz, $\parallel$ [1, 1, 1], [73L3]
$A_{\perp} = 10.1$ MHz, $\perp$ [1, 1, 1]
$A_1 = 9.1$ MHz, $\parallel$ [0 , -0.707, $+0.707$], [78S]
$A_2 = 10.4$ MHz, $\parallel$ [$+0.363$, $+0.659$, $+0.659$]
$A_3 = 8.8$ MHz, $\parallel$ [-0.932, $+0.256$, $+0.256$]

Q-tensor: nucleus ^{14}N, 3 sites
$Q_{\parallel} = -0.66$ MHz, $\parallel$ [1, 1, 1]
$Q_{\perp} = +0.33$ MHz, $\perp$ [1, 1, 1]

J-value: 0.1 MHz

A-tensor: nucleus ^{13}C, spin $S=1/2$, abundance 1.1%, 1 site
$A_{\parallel}=404$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp}=174$ MHz, $\perp$ [1. 1. 1]

A-value: nucleus ^{13}C, 3 sites
$A_{xx}=27.6$ MHz, $\parallel$ [1, 0, 0]

A-value: nucleus ^{13}C, 3 sites
$A_{xx}=19.2$ MHz, $\parallel$ [1, 0, 0]

Diamond: natural type I

Remarks: known as the "14 line" spectrum
A(^{14}N), **Q**(^{14}N), and J measured by ENDOR [73L3, 84W]
model confirmed by ODMR [80B]

Model: three-nitrogen (+vacancy) complex, see Fig. 5 (old model nitrogen-aluminum pair)

Reference: 59S2, 71S2, 73L3, 78S, 80B, 82W2, 84W

Spectrum W7 (Fig. 6)

Symmetry: monoclinic-I

Spin: $S=1/2$

g-tensor: $(g_1+g_2+g_3)/3=2.0028$

A-tensor: nucleus ^{14}N, spin $I=1$, abundance 99.63%, 1 site
measured at temperature $T=77$ K
$A_{\parallel}=123.8$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp}=87.5$ MHz, $\perp$ [1, 1, 1]

A-tensor: nucleus ^{14}N, 1 site, $T=77$ K
$A_{\parallel}=15.6$ MHz, $\parallel$ [$\bar{1}$, 1, 1]
$A_{\perp}=13.2$ MHz, $\perp$ [$\bar{1}$, 1, 1]

A-tensor: nucleus ^{14}N, spin $I=1$, abundance 99.63%, 2 sites
measured at temperature $T=450$ °C, motionally averaged spectrum, (overall defect symmetry trigonal)
$A_1=57.7$ MHz, $\parallel$ [1, 0, 0]
$A_2=50.2$ MHz, $\parallel$ [0, 1, 1]
$A_3=64.2$ MHz, $\parallel$ [0, $\bar{1}$, 1]

Diamond: natural type I, plastically deformed

Remark: anisotropic distribution of orientations

Model: (N_1CN_2) or (N_1CCN_2)-complex, close to dislocation, see Fig. 6

Reference: 73L2, 75S

Spectrum W21 (Fig. 7)

Symmetry: orthorhombic-I

Spin: $S=1/2$

g-tensor: $g_1=2.0090$, $\parallel$ [1, 0, 0]
$g_2=2.0026$, $\parallel$ [0, 1, 1]
$g_3=2.0044$, $\parallel$ [1, $\bar{1}$, 1]

A-tensor: nucleus ^{14}N, spin $I=1$, abundance 99.63%, 1 site
$A_{\parallel}=117$ MHz, $\parallel$ [0, $\bar{1}$, 1]
$A_{\perp}=0$ MHz, $\perp$ [0, $\bar{1}$, 1]

A-tensor: nucleus ^{14}N, 2 sites
$A_{\parallel}=20.4$ MHz, $\parallel$ [+0.474, +0.623, −0.623]
$A_{\perp}=12.6$ MHz, $\perp$ [+0.474, +0.623, −0.623]

Q-tensor: nucleus ^{14}N, 2 sites
$Q_{\parallel}=-3.3$ MHz, $\parallel$ [+0.474, +0.623, −0.623]
$Q_{\perp}=+1.65$ MHz, $\perp$ [+0.474, +0.623, −0.623]

Diamond: natural type Ia

Model: three-nitrogen center, see Fig. 7

Reference: 78L4, 82L2

Spectrum W24 (Fig. 8)

Symmetry: trigonal
Spin: $S=1/2$
g-tensor: $g_{\parallel}=2.0025$, $\parallel$ [1, 1, 1]
$g_{\perp}=2.0025$, $\perp$ [1, 1, 1]
A-tensor: nucleus ^{14}N, spin $I=1$, abundance 99.63%, 2 sites
$A_{\parallel}=155$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp}=81$ MHz, $\perp$ [1, 1, 1]
Diamond: natural type Ia
Model: di-nitrogen center, see Fig. 8
Reference: 81W, 83W

Spectrum W25 (Fig. 9)

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.0025$
D-tensor: $D_{\parallel}=+2732$ MHz, $\parallel$ [0, 1, 1]
$D_{\perp}=-1366$ MHz, $\perp$ [0, 1, 1]
Diamond: (green) natural type Ia, after irradiation and anneal to 600 °C
Model: (four-nitrogen + divacancy) center, see Fig. 9
Reference: 81L

Spectrum W26 (Fig. 10)

Symmetry: orthorhombic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.0025$
D-tensor: $D_{\parallel}=+2634$ MHz, $\parallel$ [0, 1, 1]
$D_{\perp}=-1317$ MHz, $\perp$ [0, 1, 1]
Diamond: (green) natural type Ia, after irradiation and anneal to 600 °C
Model: (di-nitrogen + vacancy) center, see Fig. 10
Reference: 81L

Spectrum W27

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.0025$
D-tensor: $D_{\parallel}=+1794$ MHz, $\parallel$ [+0.208, +0.692, +0.692]
$D_{\perp}=-897$ MHz, $\perp$ [+0.208, +0.692, +0.692]
Diamond: (green) natural type Ia
Model: associated with nitrogen cluster
Reference: 80W

Spectrum W28

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.0025$
D-tensor: $D_1=+1037$ MHz, $\parallel$ [+0.139, +0.700, +0.700]
$D_2=-659$ MHz, $\perp$ [+0.139, +0.700, +0.700]
$D_3=-378$ MHz, $\perp$ [+0.139, +0.700, +0.700]
Diamond: (green) natural type Ia
Model: associated with nitrogen cluster
Reference: 80W

Spectrum W30
Symmetry: trigonal
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.00$
A-tensor: nucleus ^{14}N, spin $I=1$, abundance 99.63%, 2 sites
$A_{\parallel}=137$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp}=63$ MHz, $\perp$ [1, 1, 1]
Diamond: natural type Ia, after irradiation and anneal to 450 °C
Remark: symmetry tentative
Model: center with four or more nitrogen atoms
Reference: 81L, 88L2

4.1.3.2 Acceptor-related centers

Properties of EPR spectra related to acceptor centers in diamond are compiled in Table 2.

Table 2. EPR spectra of acceptor-related centers.

Spectrum A9
Symmetry: axial
Spin: $S=1/2$
g-tensor: $g_{\parallel}\simeq 0.5$, (at $T=300$ K), $\parallel$ [1, 1, 2]
$g_{\perp}\simeq 3$, (at $T=300$ K)
Diamond: synthetic, boron doped, p-type semiconducting
Remark: g-values strongly temperature-dependent
Model: acceptor-bound hole
Reference: 72B

Spectrum A10
Symmetry: axial
Spin: $S=1/2$
g-tensor: $g_{\parallel}\simeq 0.5$, (at $T=300$ K), $\parallel$ [1, 1, 2]
$g_{\perp}\simeq 2.5$, (at $T=300$ K)
Diamond: synthetic, boron doped, p-type semiconducting
Remark: g-values strongly temperature-dependent
Model: free hole
Reference: 72B

Spectrum KY1
Symmetry: cubic
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.003$
Diamond: natural type IIb, p-type semiconducting
Model: acceptor impurity
Reference: 67B

Spectrum NL1 (Fig. 11)
Symmetry: cubic
Spin: $S=3/2$

g-value: $g=(-)1.10$
g_2-value: $g_2=(+)0.01$
ε-values: $d/b=1.55$
Diamond: natural type IIb, p-type semiconducting
Remark: observed at low temperatures ($T\approx 2$ K) under external uniaxial stress
Model: hole bound to acceptor boron
Reference: 81A1, 85A

Spectrum W32

Symmetry: trigonal
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.002$
D-tensor: $D_\parallel=+136.4$ MHz, $\parallel$ [1, 1, 1]
$D_\perp=-\ 68.2$ MHz, $\perp$ [1, 1, 1]
Diamond: natural type IIb, p-type semiconducting
Model: native center
Reference: 83L1, 87L1, 87L2

Spectrum W36

Symmetry: trigonal
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.002$
D-tensor: $D_\parallel=+103.4$ MHz, $\parallel$ [1, 1, 1]
$D_\perp=-\ 51.7$ MHz, $\perp$ [1, 1, 1]
A-tensor: nucleus ^{11}B (tentative), spin $I=3/2$, $g_n=-1.79$
$A_\parallel=8.7$ MHz, $\parallel$ [1, 1, 1]
$A_\perp=6.0$ MHz, $\perp$ [1, 1, 1]
Q-tensor: nucleus ^{11}B (tentative)
$Q_\parallel=-3.6$ MHz
$Q_\perp=+1.8$ MHz
Diamond: natural type IIb, p-type semiconducting
Model: native boron-related center
Reference: 87L1, 87L2

4.1.3.3 Transition metal impurities

Properties of EPR spectra related to transition metal impurities in diamond are compiled in Table 3.

Table 3. EPR spectra of transition metal impurities.

Spectrum E1

Symmetry: axial (tetragonal or trigonal)
Spin: $S=1/2$
g-tensor: $g_\parallel=4.117$
$g_\perp=4.43$
A-tensor: nucleus ^{59}Co, spin $I=7/2$, abundance 100%, 1 site
$A_\parallel=245$ MHz
$A_\perp=260$ MHz
Diamond: synthetic
Model: Co^{2+} impurity
Reference: 75B

Spectrum G1

g-tensor: $(g_1+g_2+g_3)/3 \simeq 3$
Diamond: synthetic
Model: transition metal impurity, nickel or iron
Reference: 62H, 67S1, 68P

Spectrum W8 (Fig. 12)

Symmetry: cubic
Spin: $S=1/2$
g-value: $g=2.031$
A-value: nucleus ^{61}Ni, spin $I=3/2$, abundance 86%, 1 site
$A=18.2$ MHz
A-tensor: nucleus ^{13}C, spin $I=1/2$, abundance 1.1%
$(A_1+A_2+A_3)/3=7.6$ MHz
Diamond: synthetic (powder), natural type Ia,b powder [77L2]
Remark: hyperfine tensor **A**(^{61}Ni) measured in synthetic enriched ^{61}Ni doped diamond [71S3]
Model: nickel impurity, oxygen-related center, damage below surface
Reference: 66L, 68P, 70B, 71S3, 77L2

Spectrum W10

Symmetry: trigonal
Spin: $S=2$
g-tensor: $(g_1+g_2+g_3)/3=2.001$
D-tensor: $D_{\parallel}=+102.8$ MHz, $\parallel$ [1, 1, 1]
$D_{\perp}=-\ 51.4$ MHz, $\perp$ [1, 1, 1]
Diamond: natural brown type IIa
Remark: earlier value spin $S=1$ incorrect
Model: interstitial neutral chromium (tentative)
Reference: 78L2, 87L1, 87L2

4.1.3.4 Irradiation defects

Properties of EPR spectra observed for irradiation-induced centers in diamond are compiled in Table 4.

Table 4. EPR spectra of irradiation-induced centers.

Spectrum A1 (Fig. 15)

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $g_1=2.0021$, $\parallel$ [0, −0.7071, +0.7071]
$g_2=2.0016$, $\parallel$ [+0.4540, +0.6300, +0.6300]
$g_3=2.0026$, $\parallel$ [−0.8910, +0.3210, +0.3210]
D-tensor: $D_1=-\ 74$ MHz, $\parallel$ [0 , −0.7071, +0.7071]
$D_2=+154$ MHz, $\parallel$ [+0.1426, +0.6999, +0.6999]
$D_3=-\ 80$ MHz, $\parallel$ [−0.9898, +0.1009, +0.1009]
A-tensor: nucleus ^{13}C, spin $I=1/2$, abundance 1.1%, 2 sites
$A_1=29.1$ MHz, $\parallel$ [0 , +0.7071, +0.7071]
$A_2=38.1$ MHz, $\parallel$ [+0.7986, −0.4254, +0.4254]
$A_3=29.1$ MHz, $\parallel$ [−0.6018, −0.5647, +0.5647]
A-tensor: nucleus ^{13}C, 2 sites
$A_1=20.4$ MHz, $\parallel$ [0 , +0.7071, +0.7071]
$A_2=26.4$ MHz, $\parallel$ [+0.7071, −0.5000, +0.5000]
$A_3=19.8$ MHz, $\parallel$ [−0.7071, −0.5000, +0.5000]

A-tensor: nucleus ^{13}C, 2 sites
$A_1 = 15.6$ MHz, $\parallel$ [0 , +0.7071, +0.7071]
$A_2 = 21.6$ MHz, $\parallel$ [+0.6561, −0.5337, +0.5337]
$A_3 = 14.4$ MHz, $\parallel$ [−0.7547, −0.4639, +0.4639]

A-tensor: nucleus ^{13}C, 4···6 sites
$(A_1 + A_2 + A_3)/3 = 11.4$ MHz

Diamond: natural type IIa, after 1···2 MeV electron irradiation at low or at room temperature, anneals out at 500 °C

Model: (impurity + interstitial carbon) complex

Reference: 71K, 85L1, 88L1

Spectrum A2

Symmetry: 100 K: monoclinic-I, 300 K: orthorhombic-I

Spin: $S = 1$

g-tensor: $g_1 = 2.0031$, $\parallel$ [1, 0, 0]
$g_2 = 2.0015$, $\parallel$ [0, 1, 1]
$g_3 = 2.0031$, $\parallel$ [0, $\bar{1}$, 1]

D-tensor: 100 K: $D_1 = -158$ MHz, $\parallel$ [+0.9981, −0.0432, −0.0432], 300 K: −170 MHz, $\parallel$ [1, 0, 0]
$D_2 = +328$ MHz, $\parallel$ [+0.0610, +0.7058, +0.7058], +352 MHz, $\parallel$ [0, 1, 1]
$D_3 = -170$ MHz, $\parallel$ [0 , −0.7071, +0.7071], −182 MHz, $\parallel$ [0, $\bar{1}$, 1]

Diamond: natural type I and II, after electron or fast neutron irradiation at low or at room temperature, anneals out at 200 °C

Remark: **D**-tensor temperature dependent

Model: three-vacancy chain, (impurity + di-interstitial) complex; new model: (impurity + interstitial) complex

Reference: 73K, 79L2, 83F1, 84L3, 88L1

Spectrum A3

Symmetry: triclinic

Spin: $S = 1$

g-tensor: $g_1 = 2.0027$, $\parallel$ [+0.88, −0.18, −0.43]
$g_2 = 2.0020$, $\perp$ [+0.88, −0.18, −0.43]
$g_3 = 2.0020$, $\perp$ [+0.88, −0.18, −0.43]

D-tensor: $D_1 = +416$ MHz, $\parallel$ [+0.8520, +0.4245, +0.3065]
$D_2 = -156$ MHz, $\parallel$ [+0.0006, +0.5846, −0.8113]
$D_3 = -260$ MHz, $\parallel$ [−0.5236, +0.6914, +0.4978]

Diamond: natural type I and II, after electron or fast neutron irradiation at low or at room temperature, anneals out at 200 °C

Model: (di-interstitial + impurity) complex; new model: (impurity + interstitial) complex

Reference: 73K, 83F1, 84L3, 88L1

Spectrum A7

Symmetry: isotropic

Spin: $S = 1$ (tentative value)

g-tensor: $(g_1 + g_2 + g_3)/3 = 2.00$

D-tensor: $D_\parallel = +112$ MHz
$D_\perp = -\ 56$ MHz

Diamond: synthetic, boron doped, after electron irradiation

Remark: resonance may be due to cavity contamination

Reference: 77B, 82F2

Spectrum A8

Symmetry: isotropic
Spin: $S=1$ (tentative value)
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: $D_{\parallel}=+62$ MHz
$D_{\perp}=-31$ MHz
Diamond: synthetic, boron doped, after electron irradiation
Remark: resonance may be due to cavity contamination
Reference: 77B, 82F2

Spectrum N6

Symmetry: monoclinic-I
Spin: $S=5/2$
g-tensor: measured at frequency 9.5 GHz
$g_1=4.4924$, $\parallel$ [0 , −0.7071, +0.7071]
$g_2=4.6684$, $\parallel$ [+0.9537, +0.2126, +0.2126]
$g_3=4.0192$, $\parallel$ [−0.3007, +0.6744, +0.6744]
D-tensor: $E/D=0.27$
g-tensor: measured at frequency 35.5 GHz
$g_1=4.0129$, $\parallel$ [0 , −0.7071, +0.7071]
$g_2=4.0274$, $\parallel$ [+0.9537, +0.2126, +0.2126]
$g_3=3.8607$, $\parallel$ [−0.3007, +0.6744, +0.6744]
Diamond: natural, after 3.5 MeV electron irradiation at room temperature
Remark: original label A-system
Model: possibly transition metal impurity (iron)
Reference: 78N

Spectrum N7

Spin: $S=5/2$
g-tensor: measured at frequency 9.5 GHz
$(g_1+g_2+g_3)/3=4.3$
D-tensor: $E/D=0.33$
Diamond: natural, after 3.5 MeV electron irradiation at room temperature
Remark: original label B-system
Model: possibly transition metal impurity (iron)
Reference: 78N

Spectrum O1 (Figs. 13 and 15)

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $g_1=2.0022$, $\parallel$ [0, $\bar{1}$, 1]
$g_2=2.0020$, $\parallel$ [1, 0, 0]
$g_3=2.0014$, $\parallel$ [0, 1, 1]
D-tensor: $D_1=-108.2$ MHz, $\parallel$ [0 , −0.707, +0.707]
$D_2=-96.8$ MHz, $\parallel$ [+1.000, −0.005, −0.005]
$D_3=+205.0$ MHz, $\parallel$ [+0.007, +0.707, +0.707]
Diamond: natural type I and IIa, after neutron or electron irradiation and annealing, anneals out at 1100 °C
Model: 4-vacancy chain, (three-vacancy + substitutional oxygen) chain, (four-vacancy + interstitial oxygen) chain
Reference: 54G, 55G, 73L1, 77L1, 77L2, 84L2, 85L1, 86L, 88L1

Spectrum O2

Symmetry: isotropic
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.0028$
Diamond: natural, after neutron irradiation
Reference: 54G, 55G, 67B

Spectrum R1 (Fig. 15)

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: $D_1=-1401$ MHz, $\parallel$ [0, $\bar{1}$, 1]
$D_2=+2802$ MHz, $\parallel$ [4, 9, 9]
$D_3=-1401$ MHz, $\parallel$ [$\bar{9}$, 2, 2]
A-tensor: nucleus ^{13}C, spin $I=1/2$, abundance 1.1%
$A_1=123$ MHz, $\parallel$ [0, $\bar{1}$, 1]
A-tensor: nucleus ^{13}C
$A_1=44.4$ MHz, $\parallel$ [0, $\bar{1}$, 1]
$A_2=39.9$ MHz, $\parallel$ [4, 9, 9]
$A_3=43.8$ MHz, $\parallel$ [$\bar{9}$, 2, 2]
A-tensor: nucleus ^{13}C
$A_1=30.6$ MHz, $\parallel$ [0, $\bar{1}$, 1]
$A_2=24.3$ MHz, $\parallel$ [4, 9, 9]
$A_3=27.3$ MHz, $\parallel$ [$\bar{9}$, 2, 2]
Diamond: natural type I and II, after 2 MeV electron or fast neutron irradiation, anneals out at 300···400 °C
Remark: original label b-system
Model: (impurity + interstitial carbon) complex
Reference: 62F, 77L1, 83L2, 85L1, 88L1

Spectrum R2 (Fig. 15)

Symmetry: tetragonal
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: $D_\parallel=+2760$ MHz, $\parallel$ [1, 0, 0]
$D_\perp=-1380$ MHz, $\perp$ [1, 0, 0]
Diamond: natural type I and II, after electron or neutron irradiation at low and at room temperature, anneals out at 400···500 °C
Remarks: excited state ≈ 37 meV above diamagnetic ground state, original label c-system
Model: (impurity + interstitial carbon) complex
Reference: 62F, 63H, 77L1, 85L1

Spectrum R3 (Fig. 15)

Symmetry: triclinic
Spin: $S=1$
g-tensor: $g_1=2.0019$, $\parallel$ [+0.758, +0.650, −0.051]
$g_2=2.0024$, $\perp$ [+0.758, +0.650, −0.051]
$g_3=2.0024$, $\perp$ [+0.758, +0.650, −0.051]
D-tensor: $D_1=+275.8$ MHz, $\parallel$ [+0.928, +0.310, +0.206]
$D_2=-123.2$ MHz, $\parallel$ [−0.242, +0.082, +0.967]
$D_3=-152.6$ MHz, $\parallel$ [+0.283, −0.947, +0.151]
Diamond: natural type I and II, after fast neutron or electron irradiation at low or at room temperature, anneals out at 500···600 °C

Remark: original label d-system
Model: (impurity + interstitial carbon) complex
Reference: 62F, 78L3, 82F2, 85L1, 88L1

Spectrum R4 (Figs. 13, 14 and 15)
Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.00$
small anisotropy detectable
D-tensor: $D_1=-104$ MHz, $\parallel$ [0, $\bar{1}$, 1]
$D_2=+310$ MHz, $\parallel$ [1, 1, 1]
$D_3=-206$ MHz, $\parallel$ [$\bar{2}$, 1, 1]
Diamond: natural type IIa, after 2 MeV electron irradiation, anneals in at 500···600 °C, anneals out at 800···900 °C
Remarks: original label e-system
identical to spectrum W6
Model: (impurity + interstitial carbon) complex; preferred model: neutral divacancy
Reference: 73L1, 77L1, 84L1, 85L1, 86L, 88L1

Spectrum R5 (Figs. 13 and 15)
Symmetry: orthorhombic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: 77 K: $D_1=-230$ MHz, 293 K: -305 MHz, $\parallel$ [1, 0, 0]
$D_2=-190$ MHz, -265 MHz, $\parallel$ [0, 1, 1]
$D_3=+420$ MHz, $+570$ MHz, $\parallel$ [0, $\bar{1}$, 1]
Diamond: natural type IIa, after 2 MeV electron irradiation, anneals in at 850 °C, anneals out at 1150 °C
Remark: D-values temperature dependent
Model: 3-vacancy chain, (divacancy + substitutional oxygen) complex, (three-vacancy + interstitial oxygen) complex
Reference: 73L1, 77L1, 85L1, 86L, 88L1

Spectrum R6 (Figs. 13 and 15)
Symmetry: orthorhombic-I
Spin: $S=1$
g-tensor: $g_1=2.0021$, $\parallel$ [1, 0, 0]
$g_2=2.0014$, $\parallel$ [0, 1, 1]
$g_3=2.0021$, $\parallel$ [0, $\bar{1}$, 1]
D-tensor: $D_1=-\ 62.2$ MHz, $\parallel$ [1, 0, 0]
$D_2=+119.7$ MHz, $\parallel$ [0, 1, 1]
$D_3=-\ 57.5$ MHz, $\parallel$ [0, $\bar{1}$, 1]
Diamond: natural type IIa, after 2 MeV electron irradiation, anneals in at 800 °C, anneals out at 1100 °C
Model: 5-vacancy chain, multi-oxygen-vacancy complex
Reference: 73L1, 77L1, 85L1, 86L, 88L1

Spectrum R7 (Fig. 15)
Symmetry: orthorhombic-I
Spin: $S=1$
g-tensor: $g_1=2.0025$, $\parallel$ [1, 0, 0]
$g_2=2.0019$, $\parallel$ [0, 1, 1]
$g_3=2.0028$, $\parallel$ [0, $\bar{1}$, 1]

D-tensor: $D_1 = -159.6$ MHz, $\parallel$ [1, 0, 0]
$D_2 = +388.1$ MHz, $\parallel$ [0, 1, 1]
$D_3 = -228.5$ MHz, $\parallel$ [0, $\bar{1}$, 1]
Diamond: natural type IIa, after 2 MeV electron irradiation, anneals in at 950 °C, anneals out at 1450 °C
Remark: earlier spin value $S=3/2$ incorrect
Model: multi-oxygen-vacancy complex (O_2V, O_2V_3)
Reference: 73L1, 85L1, 86L, 88L1

Spectrum R8 (Fig. 15)
Symmetry: orthorhombic-I
Spin: $S=1$ (or: $S=3/2$)
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: $D_1 = -168$ MHz, $\parallel$ [1, 0, 0]
$D_2 = +336$ MHz, $\parallel$ [0, 1, 1]
$D_3 = -168$ MHz, $\parallel$ [0, $\bar{1}$, 1]
(for $S=3/2$: $D_{\parallel[011]} = +168$ MHz, $D_{\perp[011]} = -84$ MHz)
Diamond: natural type IIa, after 2 MeV electron irradiation, anneals in at 900 °C, anneals out at 1400 °C
Model: multi-oxygen-vacancy complex (O_3V_3), three-vacancy chain
Reference: 73L1, 85L1, 86L

Spectrum R9
Symmetry: orthorhombic-I
Spin: $S=1$ (or: $S=3/2$)
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: $D_1 = -454$ MHz, $\parallel$ [1, 0, 0]
$D_2 = +908$ MHz, $\parallel$ [0, 1, 1]
$D_3 = -454$ MHz, $\parallel$ [0, $\bar{1}$, 1]
(for $S=3/2$: $D_{\parallel[011]} = +454$ MHz, $D_{\perp[011]} = -227$ MHz)
Diamond: natural type IIa, after 2 MeV electron irradiation, anneals in at 900 °C, anneals out at 1250 °C
Model: oxygen-vacancy complex (O_sV, O_iV_2)
Reference: 73L1, 86L

Spectrum R10 (Fig. 15)
Symmetry: orthorhombic-I
Spin: $S=1$ (or: $S=3/2$)
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: $D_1 = -35$ MHz, $\parallel$ [1, 0, 0]
$D_2 = +70$ MHz, $\parallel$ [0, 1, 1]
$D_3 = -35$ MHz, $\parallel$ [0, $\bar{1}$, 1]
(for $S=3/2$: $D_{\parallel[011]} = +35$ MHz, $D_{\perp[011]} = -17.5$ MHz)
Diamond: natural type IIa, after 2 MeV electron irradiation, anneals in at 900° C, anneals out at 1200° C
Model: oxygen-multi-vacancy complex (O_sV_5, O_iV_6)
Reference: 73L1, 85L1, 86L

Spectrum R11 (Fig. 15)
Symmetry: orthorhombic-I
Spin: $S=1$ (or: $S=3/2$)
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: $D_1 = -27$ MHz, $\parallel$ [1, 0, 0]
$D_2 = +54$ MHz, $\parallel$ [0, 1, 1]
$D_3 = -27$ MHz, $\parallel$ [0, $\bar{1}$, 1]
(for $S=3/2$: $D_{\parallel[011]} = +27$ MHz, $D_{\perp[011]} = -13.5$ MHz)

Diamond: natural type IIa, after 2 MeV electron irradiation, anneals in at 950 °C, anneals out at 1150 °C
Model: oxygen-multi-vacancy complex (O_sV_6, O_iV_7)
Reference: 73L1, 85L1, 86L

Spectrum R12 (Fig. 15)
Symmetry: trigonal
Spin: $S=1$ (or: $S=3/2$)
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: $D_{\parallel}=+104$ MHz, $\parallel$ [1, 1, 1]
$D_{\perp}=-52$ MHz, $\perp$ [1, 1, 1]
(for $S=3/2$: $D_{\parallel[111]}=+52$ MHz, $D_{\perp[111]}=-26$ MHz)
Diamond: natural type IIa, after 2 MeV electron irradiation, anneals in at 1200 °C, still present after anneal at 1650 °C
Reference: 73L1, 85L1

Spectrum R13 (Fig. 15)
Symmetry: triclinic
Spin: $S=1$
g-tensor: $g_1=2.0021$, $\parallel$ [+0.696, +0.696, +0.174]
$g_2=2.0029$, $\perp$ [+0.696, +0.696, +0.174]
$g_3=2.0029$, $\perp$ [+0.696, +0.696, +0.174]
D-tensor: $D_1=+1365$ MHz, $\parallel$ [+0.917, +0.301, +0.261]
$D_2=-515$ MHz, $\parallel$ [−0.039, −0.584, +0.811]
$D_3=-850$ MHz, $\parallel$ [+0.396, −0.754, −0.524]
Diamond: natural type IIa, after 2 MeV electron irradiation at room temperature, anneals out at 400 °C
Model: (impurity + interstitial carbon) complex
Reference: 83L2, 85L1, 88L1

Spectrum R14 (Fig. 15)
Symmetry: triclinic
Spin: $S=1$
g-tensor: $g_1=2.0018$, $\parallel$ [+0.264, +0.961, −0.087]
$g_2=2.0022$, $\parallel$ [−0.857, +0.193, −0.478]
$g_3=2.0025$, $\parallel$ [−0.443, +0.201, +0.874]
D-tensor: $D_1=+165.9$ MHz, $\parallel$ [+0.916, +0.379, +0.132]
$D_2=-78.2$ MHz, $\parallel$ [+0.140, +0.007, −0.990]
$D_3=-87.7$ MHz, $\parallel$ [+0.376, −0.925, +0.046]
Diamond: natural type IIa, after 2 MeV electron irradiation at room temperature, anneals out at 600 °C
Model: (impurity + interstitial carbon) complex
Reference: 84L2, 85L1, 88L1

Spectrum R15 (Fig. 15)
Symmetry: triclinic
Spin: $S=1$
g-tensor: $g_1=2.0018$, $\parallel$ [+0.52, +0.39, +0.76]
$g_2=2.0023$, $\perp$ [+0.52, +0.39, +0.76]
$g_3=2.0023$, $\perp$ [+0.52, +0.39, +0.76]
D-tensor: $D_1=+137.3$ MHz, $\parallel$ [+0.719, +0.633, +0.288]
$D_2=-64.2$ MHz, $\parallel$ [+0.695, −0.644, −0.319]
$D_3=-73.1$ MHz, $\parallel$ [−0.016, +0.429, −0.903]
Diamond: natural type IIa, after 2 MeV electron irradiation at room temperature, anneals out at 500 °C
Model: (impurity + interstitial carbon) complex
Reference: 84L2, 85L1, 88L1

Spectrum R16

Symmetry: low
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.00$, $|g_1-g_3|=0.0015$
Diamond: natural type IIa, after 2 MeV electron irradiation at room temperature, anneals in at 700 °C, anneals out at 900 °C
Remark: values of parameters still tentative
Reference: 84L2, 86L, 88L1

Spectrum R17 (Fig. 15)

Symmetry: triclinic
Spin: $S=1$
g-tensor: $g_1=2.0020$, $\parallel$ [+0.437, +0.686, −0.582]
$g_2=2.0026$, $\perp$ [+0.437, +0.686, −0.582]
$g_3=2.0026$, $\perp$ [+0.437, +0.686, −0.582]
D-tensor: $D_1=+245.8$ MHz, $\parallel$ [+0.932, +0.311, +0.185]
$D_2=-95.0$ MHz, $\parallel$ [+0.259, −0.930, +0.259]
$D_3=-150.8$ MHz, $\parallel$ [+0.253, −0.193, −0.948]
Diamond: natural type IIa, after 2 MeV electron irradiation at room temperature, anneals in at 700 °C, still present after anneal at 1650 °C
Reference: 84L2, 85L1, 88L1

Spectrum R18

Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.0029$
Diamond: natural type IIa, after 2 MeV electron irradiation at room temperature, anneals in at 900 °C, still present after anneal at 1650 °C
Reference: 86L

Spectrum S1

Symmetry: trigonal
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.0023$
A-tensor: nucleus ^{13}C, spin $I=1/2$, abundance 1.1%, 4 sites
$A_\parallel=13.3$ MHz, $\parallel$ [1, 1, 1]
$A_\perp=9.3$ MHz, $\perp$ [1, 1, 1]
Diamond: natural, after electron irradiation at low and at room temperature, anneals out at 800 °C
Remark: original label A-center, a-system
Model: positive or negative vacancy
Reference: 63B, 75L1, 78L2, 86L

Spectrum S2

Symmetry: trigonal
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.0023$
A-tensor: nucleus ^{14}N, spin $I=1$, abundance 99.63%, 1 site
$A_\parallel=70.7$ MHz, $\parallel$ [1, 1, 1]
$A_\perp=40.9$ MHz, $\perp$ [1, 1, 1]
Diamond: natural, after electron irradiation
Remark: original label A-center, a-system
Model: substitutional nitrogen + other defect
Reference: 63B, 73L2, 75L1, 78L2

Spectrum S3

Symmetry: isotropic
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.00238$
Diamond: natural, after electron irradiation
Remark: original label C-center
Reference: 63B, 78L2

Spectrum S4

Symmetry: isotropic
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.00234$
Diamond: natural, after electron irradiation
Remarks: two lines separated by ≈ 0.1 mT
original label B-center
Reference: 63B, 78L2

Spectrum W4

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: $D_1=-$ 74 MHz, $\parallel$ [1, 0, 0]
$D_2=+147$ MHz, $\parallel$ [0, 1, 1]
$D_3=-$ 74 MHz, $\parallel$ [0, $\bar{1}$, 1]
Diamond: natural type IIb, semiconducting, after 2 MeV electron irradiation at room temperature
Reference: 78L2, 79C

Spectrum W5

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.00$
D-tensor: $D_1=-$ 53 MHz, $\parallel$ [1, 0, 0]
$D_2=+105$ MHz, $\parallel$ [0, 1, 1]
$D_3=-$ 53 MHz, $\parallel$ [0, $\bar{1}$, 1]
Diamond: natural type IIb, semiconducting, after 2 MeV electron irradiation at room temperature
Reference: 78L2, 79C

Spectrum W6 (Fig. 14)

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $g_1=2.0024$, $\parallel$ [0, $\bar{1}$, 1]
$g_2=1.9996$, $\parallel$ [1, 1, 1]
$g_3=2.0022$, $\parallel$ [$\bar{2}$, 1, 1]
D-tensor: $D_1=-112$ MHz, $\parallel$ [0, $\bar{1}$, 1]
$D_2=+314$ MHz, $\parallel$ [1, 1, 1]
$D_3=-202$ MHz, $\parallel$ [$\bar{2}$, 1, 1]
Diamond: natural type IIa, after 2 MeV electron irradiation at low and at room temperature
Remark: identical to spectrum R4
Model: (impurity + interstitial carbon) complex
Reference: 75L2, 77L1, 78L3

Spectrum W11

Symmetry: triclinic

Spin: $S=1$ (or: $S=3/2$)

g-tensor: $(g_1+g_2+g_3)/3=2.00$

D-tensor: $D_1=872$ MHz, $\|$ [+0.695, +0.509, +0.509]
(for $S=3/2$: $D_1=436$ MHz)

Diamond: natural type Ib, after neutron irradiation, anneals out at 200 °C

Reference: 78L2, 87W

Spectrum W12

Symmetry: triclinic

Spin: $S=1$ (or: $S=3/2$)

g-tensor: $(g_1+g_2+g_3)/3=2.00$

D-tensor: $D_1=960$ MHz, $\|$ [+0.606, +0.562, +0.562]
(for $S=3/2$: $D_1=480$ MHz)

Diamond: natural type Ib, after neutron irradiation, anneals out at 400 °C

Reference: 78L2, 87W

Spectrum W13

Symmetry: monoclinic-I

Spin: $S=1$ (or: $S=3/2$)

g-tensor: $g_1=1.995$, $\|$ [0 , −0.707, +0.707]
$g_2=2.008$, $\|$ [+0.738, +0.477, +0.477]
$g_3=1.993$, $\|$ [−0.674, +0.522, +0.522]

D-tensor: $D_1=-366$ MHz, $\|$ [0 , −0.707, +0.707]
$D_2=+992$ MHz, $\|$ [+0.738, +0.477, +0.477]
$D_3=-626$ MHz, $\|$ [−0.674, +0.522, +0.522]
(for $S=3/2$: $D_1=-183$ MHz, $D_2=+496$ MHz, $D_3=-313$ MHz)

Diamond: natural type Ib, after neutron irradiation, anneals out at 400 °C

Reference: 78L2, 87W

Spectrum W14

Symmetry: monoclinic-I

Spin: $S=1$ (or: $S=3/2$)

g-tensor: $g_1=1.993$, $\|$ [0 , −0.707, +0.707]
$g_2=2.007$, $\|$ [+0.603, +0.564, +0.564]
$g_3=1.989$, $\|$ [−0.798, +0.427, +0.427]

D-tensor: $D_1=-692$ MHz, $\|$ [0 , −0.707, +0.707]
$D_2=+1085$ MHz, $\|$ [+0.603, +0.564, +0.564]
$D_3=-393$ MHz, $\|$ [−0.798, +0.427, +0.427]
(for $S=3/2$: $D_1=-346$ MHz, $D_2=+543$ MHz, $D_3=-197$ MHz)

Diamond: natural type Ib, after neutron irradiation, anneals out at 400 °C

Reference: 78L2, 87W

Spectrum W15 (Fig. 16)

Symmetry: trigonal

Spin: $S=1$

g-tensor: $g_{\|}=2.0028$, $\|$ [1, 1, 1]
$g_{\perp}=2.0028$, $\perp$ [1, 1, 1]

D-tensor: $D_{\|}=+1916$ MHz, $\|$ [1, 1, 1]
$D_{\perp}=-958$ MHz, $\perp$ [1, 1, 1]

A-tensor: nucleus ^{14}N, spin $I=1$, abundance 99.63%, 1 site
$A_{\parallel}=-2.2$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp}=-2.6$ MHz, $\perp$ [1, 1, 1]

Q-tensor: nucleus ^{14}N, 1 site
$Q_{\parallel}=-3.4$ MHz, $\parallel$ [1, 1, 1]
$Q_{\perp}=+1.7$ MHz, $\perp$ [1, 1, 1]

A-tensor: nucleus ^{13}C, spin $I=1/2$, abundance 1.1%, 3 sites
$A_{\parallel}=205$ MHz, $\parallel$ [+0.627, −0.551, −0.551]
$A_{\perp}=123$ MHz, $\perp$ [+0.627, −0.551, −0.551]

Diamond: natural type Ib, after electron or neutron irradiation, anneals in at 700 °C, still present after anneal at 1300 °C

Model: nitrogen-vacancy pair, see Fig. 16

Reference: 77L3, 78L2, 87W, 88L2

Spectrum W16

Symmetry: monoclinic-I

Spin: $S=1$ (or: $S=3/2$)

g-tensor: $g_1=2.0026$, $\parallel$ [0 , −0.707, +0.707]
$g_2=2.0029$, $\parallel$ [+0.614, +0.558, +0.558]
$g_3=2.0022$, $\parallel$ [−0.789, +0.434, +0.434]

D-tensor: $D_1=-$ 803 MHz, $\parallel$ [0 , −0.707, +0.707]
$D_2=+1652$ MHz, $\parallel$ [+0.614, +0.558, +0.558]
$D_3=-$ 849 MHz, $\parallel$ [−0.789, +0.434, +0.434]
(for $S=3/2$: $D_1=-402$ MHz, $D_2=+826$ MHz, $D_3=-425$ MHz)

Diamond: natural type Ib, after electron or neutron irradiation, anneals in at 800 °C, still present after anneal at 1400 °C

Reference: 78L2, 87W

Spectrum W17

Symmetry: triclinic

Spin: $S=1$ (or: $S=3/2$)

g-tensor: $g_1=2.0025$, $\parallel$ [+0.289, −0.819, −0.496]
$g_2=2.0033$, $\parallel$ [+0.620, +0.555, −0.555]
$g_3=2.0018$, $\parallel$ [+0.730, −0.147, +0.668]

D-tensor: $D_1=-$ 717 MHz, $\parallel$ [+0.289, −0.819, −0.496]
$D_2=+1568$ MHz, $\parallel$ [+0.620, +0.555, −0.555]
$D_3=-$ 851 MHz, $\parallel$ [+0.730, −0.147, +0.668]
(for $S=3/2$: $D_1=-359$ MHz, $D_2=+784$ MHz, $D_3=-426$ MHz)

Diamond: natural type Ib, after electron or neutron irradiation, anneals in at 900 °C, still present after anneal at 1400 °C

Reference: 78L2, 87W

Spectrum W18

Symmetry: monoclinic-I

Spin: $S=1$ (or: $S=3/2$)

g-tensor: $g_1=2.0027$, $\parallel$ [0 , −0.707, +0.707]
$g_2=2.0033$, $\parallel$ [+0.617, +0.556, +0.556]
$g_3=2.0018$, $\parallel$ [−0.787, +0.436, +0.436]

D-tensor: $D_1=-$ 666 MHz, $\parallel$ [0 , −0.707, +0.707]
$D_2=+1421$ MHz, $\parallel$ [+0.617, +0.556, +0.556]
$D_3=-$ 753 MHz, $\parallel$ [−0.787, +0.436, +0.436]
(for $S=3/2$: $D_1=-333$ MHz, $D_2=+711$ MHz, $D_3=-377$ MHz)

Diamond: natural type Ib, after electron or neutron irradiation, anneals in at 900 °C, still present after anneal at 1400 °C

Reference: 78L2, 87W

Spectrum W19

Symmetry: monoclinic-I

Spin: $S=1$ (or: $S=3/2$)

g-tensor: $g_1=2.0031$, $\|$ [0 , −0.707, +0.707]
$g_2=2.0028$, $\|$ [+0.347, +0.663, +0.663]
$g_3=2.0029$, $\|$ [−0.938, +0.245, +0.245]

D-tensor: $D_1=-333$ MHz, $\|$ [0 , −0.707, +0.707]
$D_2=+941$ MHz, $\|$ [+0.347, +0.663, +0.663]
$D_3=-608$ MHz, $\|$ [−0.938, +0.245, +0.245]
(for $S=3/2$: $D_1=-167$ MHz, $D_2=+471$ MHz, $D_3=-304$ MHz)

Diamond: natural type Ib diamond, after electron or neutron irradiation, after anneal at 900 °C

Reference: 78L2

Spectrum W20

Symmetry: monoclinic-I

Spin: $S=1/2$

g-tensor: $g_1=2.100$, $\|$ [0 , −0.707, +0.707]
$g_2=2.074$, $\|$ [+0.259, +0.683, +0.683]
$g_3=2.018$, $\|$ [−0.966, +0.183, +0.183]

Diamond: natural type Ib, after electron irradiation and anneal at 400 °C

Reference: 78L2

Spectrum W29

Symmetry: monoclinic-I

Spin: $S=1$ (or: $S=3/2$)

g-tensor: $g_1=2.002$, $\|$ [0 , −0.707, +0.707]
$g_2=2.005$, $\|$ [+0.623, −0.553, −0.553]
$g_3=1.997$, $\|$ [+0.783, +0.440, +0.440]

D-tensor: $D_1=-596$ MHz, $\|$ [0 , −0.707, +0.707]
$D_2=+907$ MHz, $\|$ [+0.623, −0.553, −0.553]
$D_3=-311$ MHz, $\|$ [+0.783, +0.440, +0.440]
(for $S=3/2$: $D_1=-298$ MHz, $D_2=+454$ MHz, $D_3=-156$ MHz)

Diamond: natural type I, after neutron or electron irradiation, anneals in above 500 °C, anneals out above 800 °C

Reference: 83F2, 87W, 88L2

Spectrum W33

Symmetry: monoclinic-I

Spin: $S=1$ (or: $S=3/2$)

g-tensor: $(g_1+g_2+g_3)/3=2.003$

D-tensor: $D_1=-1175$ MHz, $\|$ [0 , −0.707, +0.707]
$D_2=+1857$ MHz, $\|$ [+0.515, −0.606, −0.606]
$D_3=-682$ MHz, $\|$ [+0.857, +0.364, +0.364]
(for $S=3/2$: $D_1=-588$ MHz, $D_2=+929$ MHz, $D_3=-341$ MHz)

Diamond: natural and synthetic type Ib, after neutron irradiation, anneals in at 700 °C, anneals out at 1100 °C

Reference: 87W, 88L2

Spectrum W34

Symmetry: monoclinic-I
Spin: $S=1$ (or: $S=3/2$)
g-tensor: $(g_1+g_2+g_3)=2.002$
D-tensor: $D_1=-240$ MHz, $\|$ [0 , −0.707, +0.707]
$D_2=+766$ MHz, $\|$ [+0.751, −0.467, −0.467]
$D_3=-526$ MHz, $\|$ [+0.660, +0.531, +0.531]
(for $S=3/2$: $D_1=-120$ MHz, $D_2=+383$ MHz, $D_3=-263$ MHz)
Diamond: natural and synthetic type Ib, after irradiation, anneals in at 800 °C, anneals out at 1100 °C
Reference: 87W, 88L2

4.1.3.5 Ion implantation defects

Properties of EPR spectra for ion implantation-induced centers in diamond are compiled in Table 5.

Table 5. EPR spectra related to ion implantation.

Spectrum A4

Symmetry: trigonal
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.0023$
D-tensor: small
Diamond: natural type IIa, after nitrogen ion implantation
Reference: 74B2

Spectrum A5

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)=2.0023$
D-tensor: $D_1=-103.7$ MHz, $\|$ [0 , −0.7071, +0.7071]
$D_2=+300.0$ MHz, $\|$ [+0.6157, +0.5572, +0.5572]
$D_3=-196.3$ MHz, $\|$ [−0.7880, +0.4353, +0.4353]
Diamond: natural type IIa, after carbon or nitrogen implantation
Model: hexavacancy ring
Reference: 78L1

Spectrum A6

Symmetry: orthorhombic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.0023$
D-tensor: $D_1=-$ 96 MHz, $\|$ [1, 0, 0]
$D_2=+192$ MHz, $\|$ [0, 1, 1]
$D_3=-$ 96 MHz, $\|$ [0, $\bar{1}$, 1]
Diamond: natural type IIa, after carbon or nitrogen implantation
Model: multivacancy cluster
Reference: 78L1

Spectrum A11

Symmetry: isotropic
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.0023$
Diamond: natural, ion (B, C, N, Sb) implanted
Model: amorphous carbon, implantation damage
Reference: 74B1, 75M, 78L1, 79T

4.1.3.6 Miscellaneous centers

Properties of EPR spectra for miscellaneous centers in diamond are compiled in Table 6.

Table 6. EPR spectra of miscellaneous centers.

Spectrum L1

Spin: $S=1/2$
g-tensor: $g_1=2.000$
$g_2=2.000$
$g_3=2.000$
A-tensor: nucleus ^{29}Si, spin $I=1/2$, abundance 4.7%
$A_1=196$ MHz
$A_2=232$ MHz
$A_3=251$ MHz
Diamond: natural type Ia
Model: native (silicon + impurity) center (tentative)
Reference: 77M

Spectrum N2

Symmetry: isotropic
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.003$
Diamond: natural, plastically deformed
Model: dislocation-related center
Reference: 75S

Spectrum N5

Symmetry: axial
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.0027$
A-tensor: nucleus ^{13}C, spin $I=1/2$, abundance 1.1%, 1···2 sites
$A_{\parallel}=667$ MHz
$A_{\perp}=336$ MHz
Diamond: natural type I, crushed
Model: surface center
Reference: 67S2

Spectrum TI1

Symmetry: isotropic
Spin: $S=1/2$
g-tensor: $(g_1+g_2+g_3)/3=2.0027$

Diamond: pulverized
Model: surface damage
Reference: 61W, 67B, 67S2

Spectrum W1

Symmetry: orthorhombic-I
Spin: $S=1$
g-tensor: $g_1=2.0029$, $\parallel$ [1, 0, 0]
$g_2=2.0026$, $\parallel$ [0, 1, 1]
$g_3=2.0029$, $\parallel$ [0, $\bar{1}$, 1]
D-tensor: $D_1=-217$ MHz, $\parallel$ [1, 0, 0]
$D_2=+374$ MHz, $\parallel$ [0, 1, 1]
$D_3=-157$ MHz, $\parallel$ [0, $\bar{1}$, 1]
Diamond: natural type Ib
Remark: possibly produced by geological irradiation
Model: native center
Reference: 71S1, 73L1

Spectrum W2

Symmetry: orthorhombic-I
Spin: $S=1$
g-tensor: $g_1=2.0030$, $\parallel$ [1, 0, 0]
$g_2=2.0027$, $\parallel$ [0, 1, 1]
$g_3=2.0030$, $\parallel$ [0, $\bar{1}$, 1]
D-tensor: $D_1=-206$ MHz, $\parallel$ [1, 0, 0]
$D_2=+411$ MHz, $\parallel$ [0, 1, 1]
$D_3=-206$ MHz, $\parallel$ [0, $\bar{1}$, 1]
Diamond: natural type Ib
Remark: possibly produced by geological irradiation
Model: native center
Reference: 71S1, 73L1

Spectrum W3

Symmetry: orthorhombic-I
Spin: $S=1$
g-tensor: $g_1=2.0029$, $\parallel$ [1, 0, 0]
$g_2=2.0026$, $\parallel$ [0, 1, 1]
$g_3=2.0029$, $\parallel$ [0, $\bar{1}$, 1]
D-tensor: $D_1=-230$ MHz, $\parallel$ [1, 0, 0]
$D_2=+460$ MHz, $\parallel$ [0, 1, 1]
$D_3=-230$ MHz, $\parallel$ [0, $\bar{1}$, 1]
Diamond: natural type Ib
Remark: possibly produced by geological irradiation
Model: native center
Reference: 71S1, 73L1

Spectrum W9

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=2.002$
D-tensor: $D_{\parallel}=+132$ MHz, $\parallel$ [0, $\bar{1}$, 1]
$D_{\perp}=-\ 66$ MHz, $\perp$ [0, $\bar{1}$, 1]
Diamond: natural type IIa, brown

Model: native center
Reference: 78L2, 87L1, 87L2

Spectrum W22

Symmetry: monoclinic-I
Spin: $S=1/2$
g-tensor: $g_1=2.1096$, $\parallel$ [0 , −0.707, +0.707]
$g_2=2.0817$, $\parallel$ [+0.940, +0.242, +0.242]
$g_3=2.0216$, $\parallel$ [−0.342, +0.664, +0.664]
Diamond: natural type Ib
Model: related to oxygen (tentative)
Reference: 79L1

Spectrum W23

Symmetry: monoclinic-I
Spin: $S=1/2$
g-tensor: $g_1=2.1121$, $\parallel$ [0 , −0.707, +0.707]
$g_2=2.0833$, $\parallel$ [+0.940, +0.242, +0.242]
$g_3=2.0197$, $\parallel$ [−0.342, +0.664, +0.664]
Diamond: natural type Ib
Model: related to oxygen (tentative)
Reference: 79L1

Spectrum W31

Symmetry: trigonal
Spin: $S=1/2$
g-tensor: $g_{\parallel}=2.0020$, $\parallel$ [1, 1, 1]
$g_{\perp}=2.0025$, $\perp$ [1, 1, 1]
A-tensor: nucleus ^{33}S, spin $I=3/2$, abundance 0.75%, 1 site
$A_{\parallel}=1029$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp}=1034$ MHz, $\perp$ [1, 1, 1]
A-tensor: nucleus ^{13}C, spin $I=1/2$, abundance 1.1%, 4 sites
$A_{\parallel}=70.6$ MHz, $\parallel$ [+0.485, +0.618, +0.618]
$A_{\perp}=45.1$ MHz, $\perp$ [+0.485, +0.618, +0.618]
A-tensor: nucleus ^{13}C, 6 sites
$A_{\parallel}=14.9$ MHz, $\parallel$ [1, 1, 1]
$A_{\perp}=9.8$ MHz, $\perp$ [1, 1, 1]
A-tensor: nucleus ^{13}C, 12 sites
$(A_1+A_2+A_3)/3=4.8$ MHz
Diamond: natural type Ib, after heating to above 300 °C in dark
Model: (interstitial) S^+
Reference: 82W1, 86W

Spectrum W35

Symmetry: monoclinic-I
Spin: $S=1$
g-tensor: $(g_1+g_2+g_3)/3=1.998$
D-tensor: $D_1=+202.7$ MHz, $\parallel$ [0, $\bar{1}$, 1]
$D_2=-30.6$ MHz, $\perp$ [0, $\bar{1}$, 1]
$D_3=-172.1$ MHz, $\perp$ [0, $\bar{1}$, 1]
Diamond: natural type IIa, brown
Model: native center
Reference: 87L1, 87L2

Figures for 4.1.3

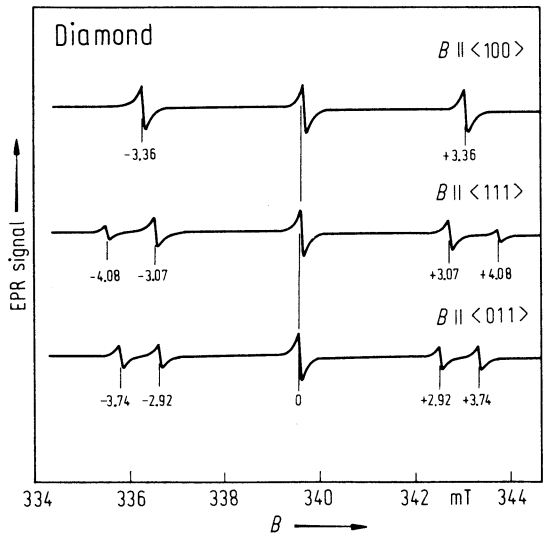

Fig. 1. Diamond. EPR spectrum P1 for magnetic field $\boldsymbol{B}$ parallel to the three main crystallographic directions ⟨100⟩, ⟨111⟩ and ⟨011⟩ [59S1].

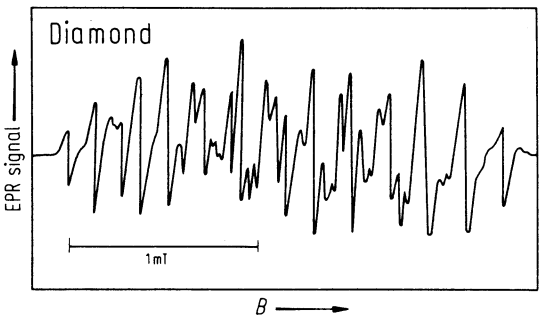

Fig. 2. Diamond. EPR spectrum P2, the "14 line" spectrum, for $\boldsymbol{B}\|\langle 100\rangle$ [71S2].

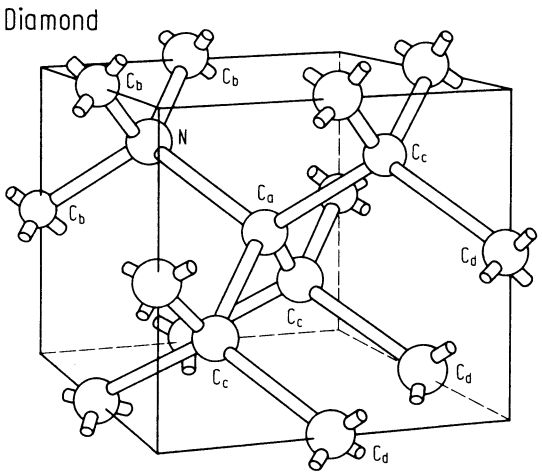

Fig. 4. Diamond. Atomic structure model for the P1 center [78L2].

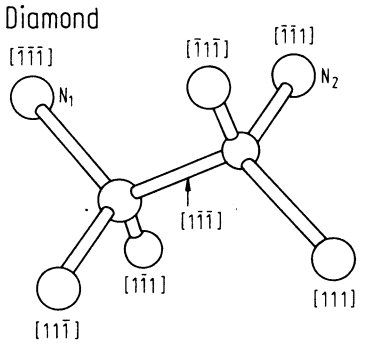

Fig. 3. Diamond. Atomic structure model for the N1 center [85L2].

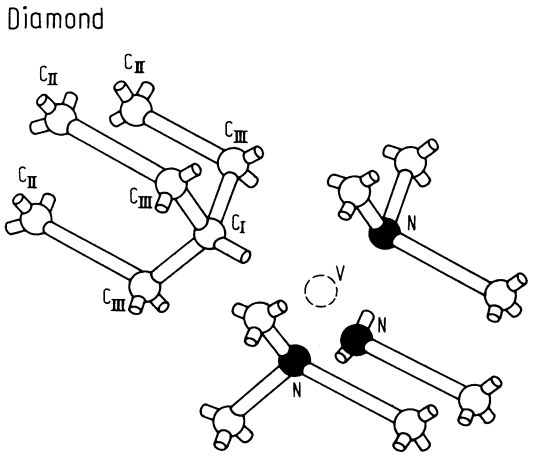

Fig. 5. Diamond. Atomic structure model for the P2 center [78S].

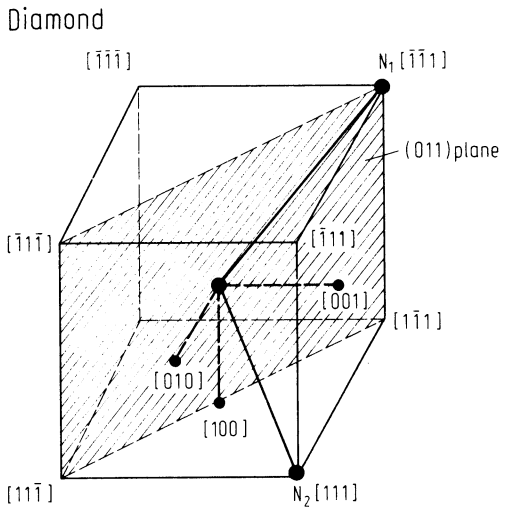

Fig. 6. Diamond. Atomic structure model for the W7 center [73L2].

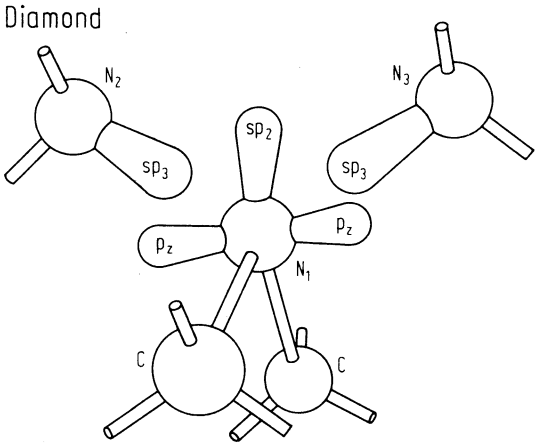

Fig. 7. Diamond. Atomic structure model for the W21 center [82L2].

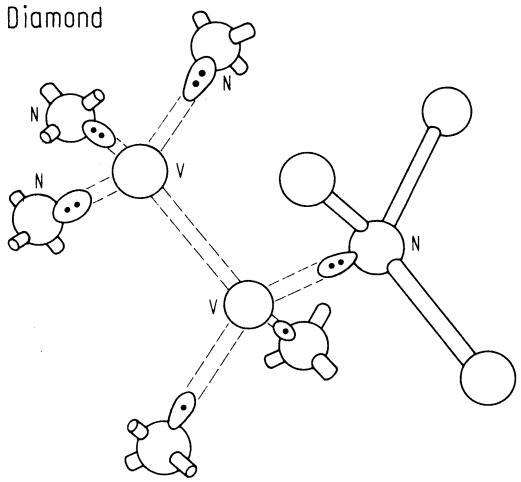

Fig. 9. Diamond. Atomic structure model for the W25 center [81L].

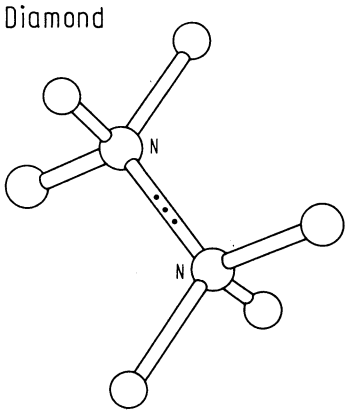

Fig. 8. Diamond. Atomic structure model for the W24 center [83W].

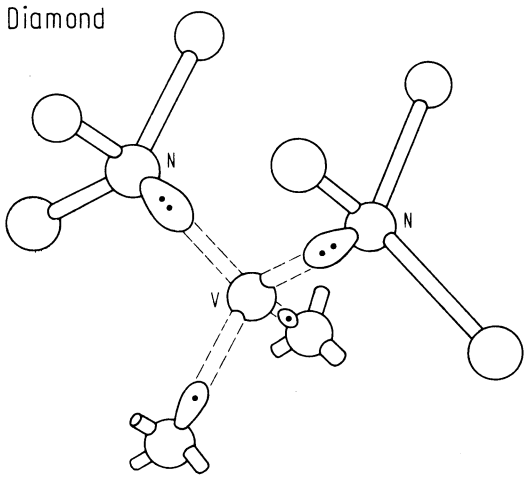

Fig. 10. Diamond. Atomic structure model for the W26 center [81L].

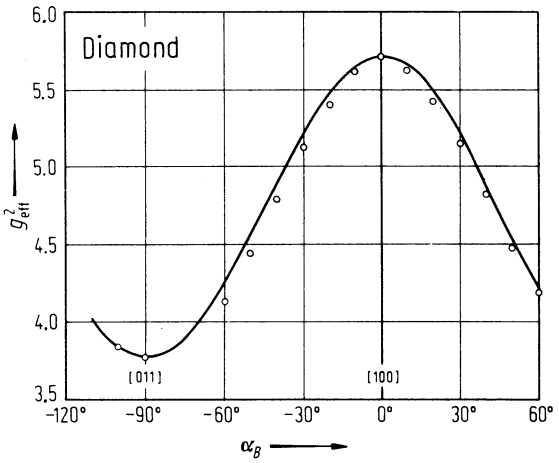

Fig.11. Diamond. Angular dependence of the effective g^2-value of spectrum NL1 for rotation angle α_B of the magnetic field $\boldsymbol{B}$ in the $(0\bar{1}1)$-plane [81A1].

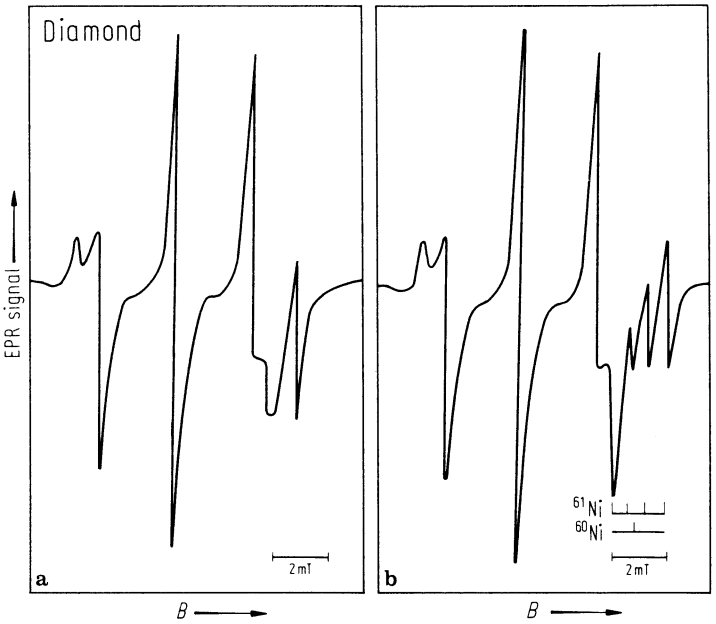

Fig. 12a, b. Diamond. EPR spectrum W8 superimposed upon the P1 spectrum; (a) synthetic diamond grown with natural nickel catalyst, (b) diamond grown with nickel enriched to 86% in the magnetic ^{61}Ni isotope with nuclear spin $I=3/2$ [71S3].

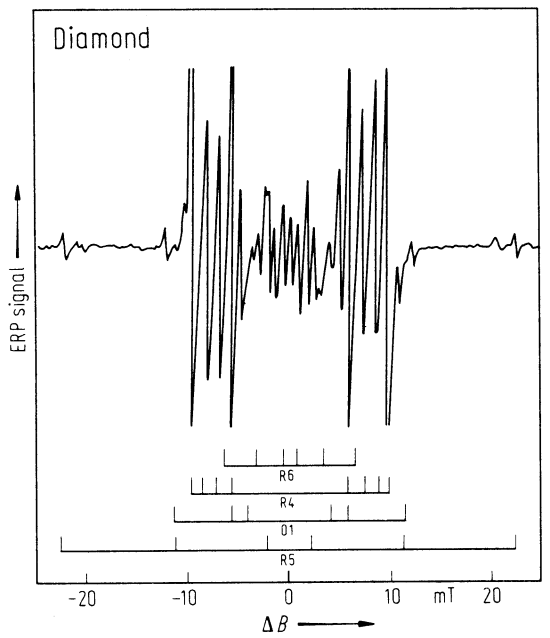

Fig. 13. Diamond. EPR spectra for $\boldsymbol{B}\|\langle 011\rangle$ produced in type IIa diamond by electron irradiation and anneal to 800 °C. Calculated line positions for the O1, R4, R5 and R6 spectra are indicated [77L1].

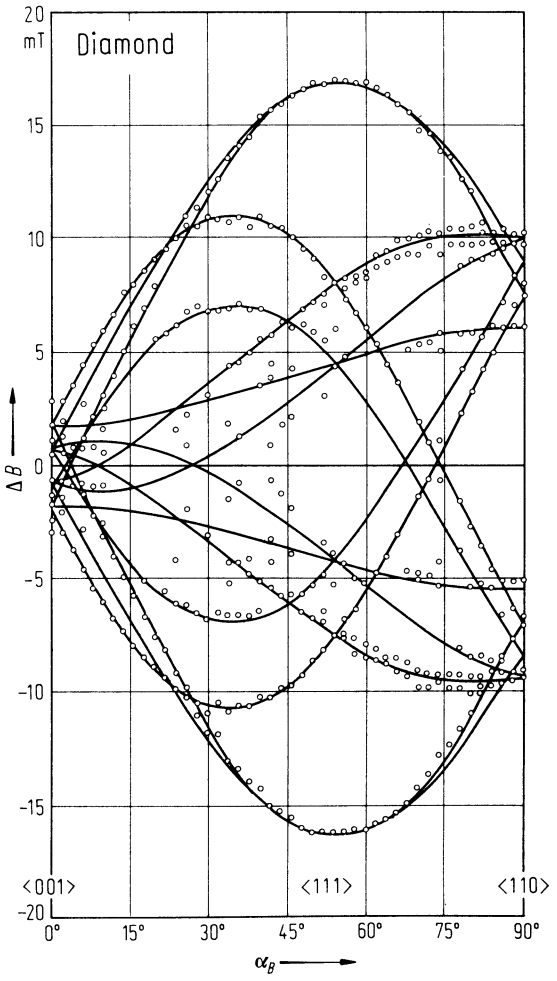

Fig. 14. Diamond. Angular variation or the resonance field for rotation angle α_B of $\boldsymbol{B}$ in the $\langle 011\rangle$-plane for spectrum R4 ≡ W6 [77L1].

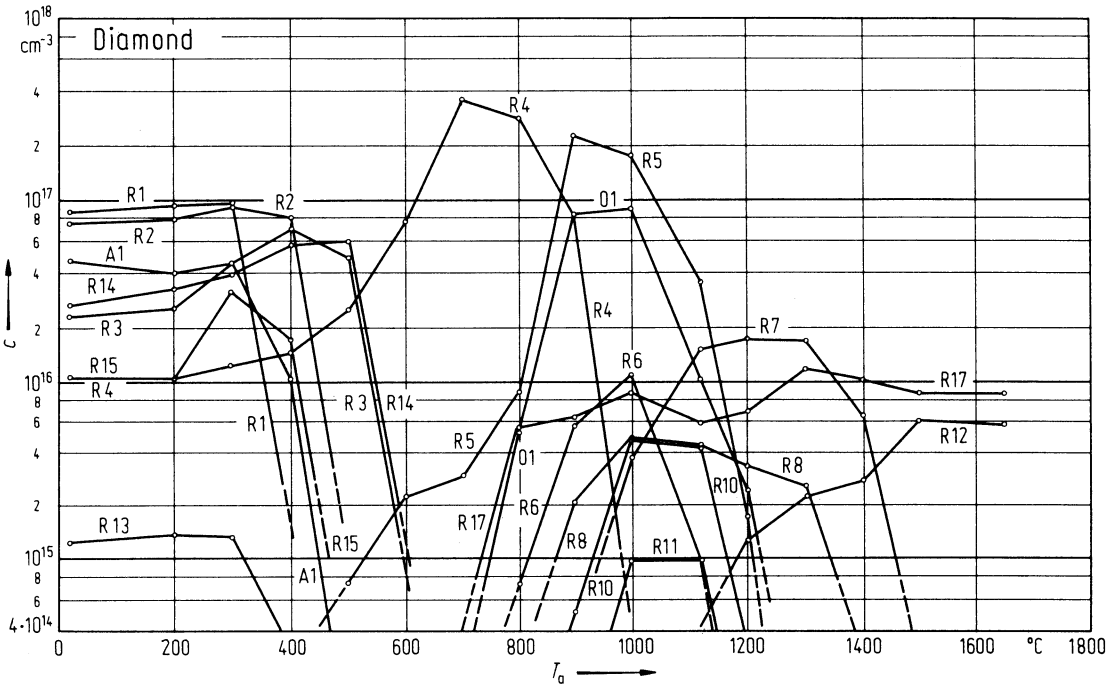

Fig. 15. Diamond. Characteristics of 30-minutes isochronal annealing-in and annealing-out of EPR spectra produced by electron irradiation in type IIa diamond [85L1]. (c: defect concentration, T_a: annealing temperature).

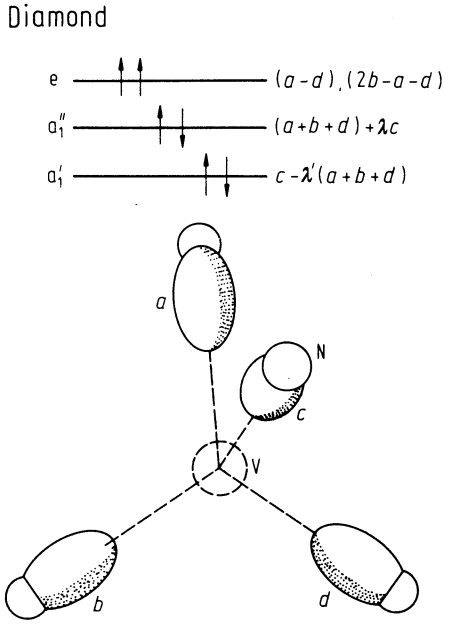

Fig. 16. Diamond. One-electron LCAO orbitals and possible energy level scheme for the nitrogen-vacancy pair, accounting for the trigonal symmetry and spin $S=1$ of the W15 spectrum [77L3].

References for 4.1.3

54G Griffiths, J.H.E., Owen, J., Ward, I.M: Nature **173** (1954) 439.

55G Griffiths, J.H.E., Owen, J., Ward, I.M.: Report of the Conference on Defects in Crystalline Solids, London: Physical Society **1955,** p. 81.

59S1 Smith, W.V., Sorokin, P.P., Gelles, I.L., Lasher, G.J.: Phys. Rev. **115** (1959) 1546.

59S2 Smith, W.V., Gelles, I.L., Sorokin, P.P.: Phys. Rev. Lett. **2** (1959) 39.

61W Walters, G.K., Estle, T.L.: J. Appl. Phys. **32** (1961) 1854.

62F Faulkner, E.A., Lomer, J.N.: Philos. Mag. **7** (1962) 1995.

62H Huggins, C.M., Cannon, P.: Nature **194** (1962) 829.

63B Baldwin jr., J.A.: Phys. Rev. Lett. **10** (1963) 220.

63H Harris, E.A., Owen, J., Windsor, C.: Bull. Am. Phys. Soc., Ser. II, **8** (1963) 252.

65D Dyer, H.B., Raal, F.A., du Preez, L., Loubser, J.H.N.: Philos. Mag. **11** (1965) 763.

65L Loubser, J.H.N., du Preez, L.: Br. J. Appl. Phys. **16** (1965) 457.

66C Cook R.J., Whiffen, D.H.: Proc. R. Soc. London Ser. A **295** (1966) 99.

66L Loubser, J.H.N., van Ryneveld, W.P.: Nature **211** (1966) 517.

67B Bell, M.D., Leivo, W.J.: J. Appl. Phys. **38** (1967) 337.

67S1 Smith, M.J.A., Angel, B.R.: Philos. Mag. **15** (1967) 783.

67S2 Samsonenko, N.D., Sobolev, E.V.: Pis'ma Zh. Eksp. Teor. Fiz. **5** (1967) 304; JETP Lett. (English Transl.) **54** (1967) 250.

68P Podzyarei, G.A., Zaritskii, I.M.: Teor. Eksp. Khim. **4** (1968) 281; Theor. Exp. Chem. USSR (English Transl.) **4** (1968) 183.

69S Shcherbakova, M.Ya., Sobolev, E.V., Samsonenko, N.D., Aksenov, V.K.: Fiz. Tverd. Tela Leningrad **11** (1969) 1364; Sov. Phys. Solid State (English Transl.) **11** (1969) 1104.

70B Bratashevskii, Yu.A., Litvin, Yu.A., Samsonenko, N.D., Sobolev, E.V.: Izv. Akad. Nauk SSSR Neorg. Mater. **6** (1970) 368.

70K Klingsporn, P.E., Bell, M.D., Leivo, W.J.: J. Appl. Phys. **41** (1970) 2977.

71K Kim, Y.M., Watkins, G.D.: J. Appl. Phys. **42** (1971) 722.

71S1 Szendrei, T.: Solid State Commun. **9** (1971) 313.

71S2 Shcherbakova, M.Ya., Soboleva, E.V., Samsonenko, N.D., Nadolinnyi, V.A., Schastnev, P.V., Semenov, A.G.: Fiz. Tverd. Tela Leningrad **13** (1971) 341; Sov. Phys. Solid State (English Transl.) **13** (1971) 281.

71S3 Samoilovich, M.I., Bezrukov, G.N., Butuzov, V.P.: Pis'ma Zh. Eksp. Teor. Fiz. **14** (1971) 551; JETP Lett. (English Transl.) **14** (1971) 379.

71S4 Shul'man, L.A., Podzyarei, G.A., Nachal'naya, T.A.: Ukr. Fiz. Zh. **16** (1971) 371.

72B Bourgoin, J.C., Brosious, P.R., Kim, Y.M., Corbett, J.W., Chrenko, R.M.: Philos. Mag. **26** (1972) 1167.

72S Shcherbakova, M.Ya., Sobolev, E.V., Nadolinnyi, V.A.: Dokl. Akad. Nauk SSSR **204** (1972) 851; Sov. Phys. Dokl. (English Transl.) **17** (1972) 513.

73K Kim, Y.M., Lee, Y.H., Brosious, P., Corbett, J.W.: Radiation Damage and Defects in Semiconductors, London: Institute of Physics **1973,** p. 202.

73L1 Lomer, J.N., Wild, A.M.A.: Radiat. Eff. **17** (1973) 37.

73L2 Loubser, J.H.N., Wright, A.C.J.: J. Phys. D **6** (1973) 1129.

73L3 Loubser, J.H.N., Wright, A.C.J.: Diamond Research, Suppl. to Ind. Diamond Rev. **1973,** p. 16.

74B1 Brosious, P.R., Corbett, J.W., Bourgoin, J.C.: Phys. Status Solidi (a) **21** (1974) 677.

74B2 Brosious, P.R., Lee, Y.H., Corbett, J.W., Cheng, L.J.: Phys. Status Solidi (a) **25** (1974) 541.

74S Strnisa, F.V., Corbett, J.W.: Cryst. Lattice Defects **5** (1974) 261.

75B Bagdasaryan, V.S., Markosyan, E.A., Matosyan, M.A., Torosyan, O.S., Sharoyan, E.G.: Fiz. Tverd. Tela Leningrad **17** (1975) 1518; Sov. Phys. Solid State (English Transl.) **17** (1975) 991.

75K Klyuev, Yu.A., Nepsha, V.I., Naletov, A.M.: Fiz. Tverd. Tela Leningrad **16** (1974) 3259; Sov. Phys. Solid State (English Transl.) **16** (1975) 2118.

75L1 Loubser, J.H.N.: Cambridge, UK: Diamond Conference **1975,** paper no. 5.

75L2 Lomer, J.N., Welbourn, C.M.: Cambridge, UK: Diamond Conference **1975,** paper no. 9.

75M Morhange, J.-F., Beserman, R., Bourgoin, J.C.: Jpn. J. Appl. Phys. **14** (1975) 544.

75S Shcherbakova, M.Ya., Sobolev, E.V., Nadolinnyi, V.A., Aksenov, V.K.: Dokl. Akad. Nauk SSSR **225** (1975) 566; Sov. Phys. Dokl. (English Transl.) **20** (1975) 725.

77B Brosious, P.R., Corbett, J.W., Bourgoin, J.C.: J. Phys. Paris **38** (1977) 459.

77L1 Lomer, J.N., Welbourn, C.M.: Radiation Effects in Semiconductors 1976, Bristol: Institute of Physics **1977,** p. 339.

77L2 Loubser, J.H.N.: Solid State Commun. **22** (1977) 767.
77L3 Loubser, J.H.N., van Wijk, J.A.: Diamond Research, Suppl. to Ind. Diamond Rev. **1977,** p. 11.
77M McNeil, D.A.C., Symons, M.C.R.: J. Phys. Chem. Solids **38** (1977) 397.
78L1 Lee, Y.H., Brosious, P.R., Corbett, J.W.: Phys. Status Solidi (a) **50** (1978) 237.
78L2 Loubser, J.H.N., van Wijk, J.A.: Rep. Prog. Phys. **41** (1978) 1201.
78L3 Lomer, J.N., Welbourn, C.M.: Philos. Mag. A **37** (1978) 639.
78L4 Loubser, J.H.N., van Wijk, J.A., Welbourn, C.M.: Oxford, UK: Diamond Conference **1978,** p. 43.
78N Nadolinnyi, V.A., Shcherbakova, M.Ya., Sobolev, E.V.: Zh. Strukt. Khim. **19** (1978) 377; J. Struct. Chem. USSR (English Transl.) **19** (1978) 327.
78S Shcherbakova, M.Ya., Nadolinnyi, V.A., Sobolev, E.V.: Zh. Strukt. Khim. **19** (1978) 305; J. Struct. Chem. USSR (English Transl.) **19** (1978) 261.
78W Welbourn, C.M.: Solid State Commun. **26** (1978) 255.
79C Clark, C.D., Mitchell, E.W.J., Parsons, B.J.: The Properties of Diamond, Field, J.E. (ed), London: Academic Press **1979,** p. 23.
79L1 Loubser, J.H.N., van Wijk, J.A.: Cambridge, UK: Diamond Conference **1979,** p. 23.
79L2 Lomer, J.N., Marriott, D.: Defects and Radiation Effects in Semiconductors 1978, Bristol: Institute of Physics **1979,** p. 341.
79T Talmi, A., Beserman, R., Braunstein, G., Bernstein, T., Kalish, R.: Defects and Radiation Effects in Semiconductors 1978, Bristol: Institute of Physics **1979,** p. 347.
80A Ammerlaan, C.A.J., Burgemeister, E.A.: Ind. Diamond Rev. **40** (1980) 128.
80B Barklie, R.C., Guven, J., Henderson, B.: Bristol, UK: Diamond Conference **1980,** p. 52.
80W van Wijk, J.A., Loubser, J.H.N.: Bristol, UK: Diamond Conference **1980,** p. 90.
81A1 Ammerlaan, C.A.J.: Defects and Radiation Effects in Semiconductors 1980, Bristol: Institute of Physics **1981,** p. 81.
81A2 Ammerlaan, C.A.J., Burgemeister, E.A.: Phys. Rev. Lett. **47** (1981) 954.
81B Barklie, R.C., Guven, J.: J. Phys. C **14** (1981) 3621.
81L Loubser, J.H.N., van Wijk, J.A.: Reading, UK: Diamond Conference **1981,** p. 35.
81W van Wijk, J.A., Loubser, J.H.N.: Reading, UK: Diamond Conference **1981,** p. 29.
82F1 Flint, I.T., Lea-Wilson, M.A., Lomer, J.N.: Oxford, UK: Diamond Conference **1982,** p. 141.
82F2 Flint, I.T., Lomer, J.N.: Oxford, UK: Diamond Conference **1982,** p. 142.
82L1 Loubser, J.H.N.: Oxford, UK: Diamond Conference **1982,** p. 135.
82L2 Loubser, J.H.N., van Wijk, J.A., Welbourn, C.M.: J. Phys. C **15** (1982) 6031.
82W1 van Wijk, J.A., Loubser, J.H.N.: Oxford, UK: Diamond Conference **1982,** p. 131.
82W2 van Wijk, J.A.: J. Phys. C **15** (1982) L981.
83F1 Flint, I.T., Lomer, J.N.: Physica **116B** (1983) 183.
83F2 Field, J.E.: Diamond: Properties and Definitions, Cambridge, UK: Cavendish Laboratory **1983.**
83L1 Loubser, J.H.N., van Wijk, J.A.: Cambridge, UK: Diamond Conference **1983,** p. 130.
83L2 Lea-Wilson, M.A., Lomer, J.N.: Cambridge, UK: Diamond Conference **1983,** p. 136.
83W van Wijk, J.A., Loubser, J.H.N.: J. Phys. C **16** (1983) 1501.
84L1 Lea-Wilson, M.A., Lomer, J.N.: Bristol, UK: Diamond Conference **1984,** p. 61.
84L2 Lea-Wilson, M.A., Lomer, J.N.: Bristol, UK: Diamond Conference **1984,** paper P8.
84L3 Lea-Wilson, M.A., Lomer, J.N.: Bristol, UK: Diamond Conference **1984,** paper P9.
84W van Wijk, J.A., Loubser, J.H.N.: Bristol, UK: Diamond Conference **1984,** p. 60.
85A Ammerlaan, C.A.J., van Kemp, R.: J. Phys. C **18** (1985) 2623.
85L1 Lea-Wilson, M.A., Lomer, J.N.: Reading, UK: Diamond Conference **1985,** paper P5.
85L2 Loubser, J.H.N., van Wijk, J.A.: Mater. Res. Soc. Symp. Proc. **46** (1985) 587.
86L Lea-Wilson, M.A., Lomer, J.N.: Royal Holloway, UK: Diamond Conference **1986,** p. 147.
86W van Wijk, J.A., Loubser, J.H.N.: Mater. Sci. Forum **10–12** (1986) 923.
87L1 Loubser, J.H.N., van Wijk, J.A.: Oxford, UK: Diamond Conference **1987,** paper P11.
87L2 Loubser, J.H.N., van Wijk, J.A.: S. Afr. J. Phys. (S. Africa) **10** (1987) 165.
87W van Wijk, J.A., Woods, G.S.: Oxford, UK: Diamond Conference **1987,** paper 10.
88B Baker, J.M., Loubser, J.H.N., Newton, M.E.: Cambridge, UK: Diamond Conference **1988.**
88L1 Lea-Wilson, M.A.: Ph. D. Thesis, Reading, UK: Reading University **1988.**
88L2 Loubser, J.H.N.: private communication **1988.**