J. Phys.: Condens. Matter 2 (1990) 2875–2928. Printed in the UK

REVIEW ARTICLE

The spectroscopy of crystal defects: a compendium of defect nomenclature

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Received 28 July 1989

Abstract. We bring together tables of current defect nomenclature and a summary of the rules actually practised (rather than idealised schemes) in choosing such labels for signals obtained with a range of spectroscopies. As well as providing a source of reference for the user lost in a maze of labels, the compilation also indicates parallels between similar defect species in very different systems (e.g. ice and quartz), even though the relationships may be far from obvious from the labels. The systems considered are all non-metals, namely ionic crystals (including oxides), silica, semiconductors (e.g. III–V and tetrahedrally coordinated II–VI), valence crystals (e.g. diamond, c-Si, a-Si) and other special hosts like ice and conducting polymers.

1. Introduction

The study of defects in solids includes many ideas and results that are of broad interest. There are parallels between the behaviour of transition-metal ions and semiconductor vacancies, between alkali halides and silicon dioxide, and even between conventional polar crystals and the important yet less-studied defects in ice. Yet there are real obstacles to the gains of work in one field helping the development of another. We have noticed this especially in the way older results for ionic crystals have been rediscovered in a semiconductor context, and the way that new results for semiconductors have been slow to reach those for other types of solids.

One of the obstacles is, at first sight, a trivial one: defect nomenclature. Here there are several components, notably the need for an experimenter to give a label to a signal before the full details of the defect responsible can be determined. Another problem is that there are several sets of 'systematic' notation. Clearly, systematic notation is a worthy object, but it is hard to avoid a bias to a particular type of material, or to a type of experiment (so that spin resonance concentrates on how one describes unpaired spins, whereas solid-state chemists may prefer to work with net charge). Nor are standard texts enough. Despite occasional valiant efforts to explain the ideas of these systems (see e.g. the appendix of Hayes and Stoneham 1985), all texts concentrate on a sample of possible

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0953-8984/90/132875 + 54 $03.50

defects rather than on their names. Likewise, most reviews are rightly concerned with the extent and accuracy of data rather than with the prudence with which authors have used labels.

We decided that different fields of defect studies could gain from cross-fertilisation by a fairly simple step, namely a systematic list of defect labels. A semiconductor scientist will be able to see at a glance that an H centre in an alkali halide is an interstitial halogen, whereas hydrogen defects are usually U centres (the U having one of several suffices). Only when one does have a fairly comprehensive list like this can one expect to produce a good general scheme, but such schemes are outside our present aims.

2. General points

We have indicated already the distinction between 'signals', i.e. the energy of some transition or a derived parameter like a g-factor, and 'models', i.e. the particular atomic species, their positions in the host lattice and their charge states, which are invoked to explain a signal or set of signals. These lead to quite different types of defect label, which is one reason why universal schemes are often unsatisfactory.

Consider first the schemes proposed to label observed *signals*. Here there are three main approaches.

Historical labels. These label a particular optical band or spin resonance transition for reasons that made sense to the original experimenter. The language in which the label made sense need not be English, e.g. the F centre in alkali halides (an electron at an anion vacancy) was so-called from the German word 'Farben', meaning colour, from the observed effect of these defects on the crystal properties. Other examples of historical labels are the M, R and N centres (essentially aggregates of F centres, involving electrons trapped at anion vacancies). Hole centres in alkali halides are traditionally V centres (with various suffices); the GR1 centre in diamond, now known to be due to the neutral vacancy, is so-called because it is produced by 'general radiation'. Problems arise with this scheme because the letters have other meanings, notably chemical ones: the F centre is not related to fluorine, the H centre is not related to hydrogen (but the U centres do involve hydrogen, not uranium) and the V centres are unrelated to vanadium. There is clearly little point in retaining a historical label unless its use has become so widespread that change would be harmful, and indeed we shall give a later example of a case where changes have simply caused confusion.

Given the possible confusions of labels for specific ions and for vacancies or interstitials, we shall use *lower-case* symbols (v for vacancies and i for interstitials) in these tables; subscripts will be added in an obvious way (e.g. v_{Ga} is a gallium vacancy) as necessary. This particular usage is non-standard, but is a simple and useful way of avoiding confusion.

Energy labels. These can be quantitative ('the line at 2.13 eV' or perhaps 'the thermoluminescence peak at 283 K') or qualitative. Examples of qualitative labels occur in deep-level transient spectroscopy (DLTS) and in thermal annealing studies. In DLTS one might find electron traps labelled E1, E2, . . . in order of increasing electron binding, and hole traps labelled H1, H2, . . . in order of increasing hole binding. In thermal anneals, there are often distinct stages, perhaps after radiation damage. Thus the defect that moves at stage I is the 'stage I defect', and so on.

Laboratory labels. These provide perhaps the most convenient labels, easily chosen, avoiding duplication, and easily identified with a model when that is appropriate. The scheme seems to have been used first by G D Watkins in his work on radiation-induced defects in silicon. It works as follows. Each laboratory gives itself a prefix (e.g. HAR for Harwell, or SC for Santa Cruz) and then numbers signals of a given type chronologically as they are found. At a later stage one might learn that the optical line labelled HAR8 is a donor–interstitial pair, for instance, and comes from the same defect as the SC27 spin resonance signal. The method has been used primarily for defects in silicon (where the G2 centre is a negatively charged vacancy, the B1, G3 and G4 centres are oxygen–vacancy complexes, the G9 centre an aluminium–vacancy pair, and so on) and diamond, though it can be generalised without problems. We recommend all laboratories to adopt this scheme initially, rather than try to speculate on a model too firmly at an early stage.

Consider next the labels for known or proposed defect *models*. We first consider crystalline solids, where there are fewer complications than for amorphous structures. We find at once that there is a choice to be made, and indeed a choice that prevents general schemes being universally satisfactory: Is the user mainly interested in the number of *carriers* (as in almost all electronic measurement, like spin resonance or electronic transport) or in the *net charge* of the defect, as in many areas of solid-state chemistry?

Quantum-chemical labels. Here the carriers alone are the observed active participants, the net charge being secondary. One convenient way—especially for the family of donors, acceptors, pairs, bound excitons, etc., in semiconductors—is to write the core as ⊕, ⓪, ⊖, etc., merely giving its net charge, but indicating the carriers (e, h) explicitly. Carriers and cores bound together are enclosed in square brackets, e.g. [⊕ e] is a simple neutral donor, a simple neutral acceptor is [⊖ h] and an exciton bound to an isovalent defect is [⓪ eh]; if the electron is excited, it would be written as [⓪ e*h], etc. This approach is very useful for writing series of electronic processes unambiguously, e.g. when one wishes to develop a Born–Haber cycle.

Kröger–Vink notation. This establishes a notation that defines net charge relative to a defect-free host. It does not distinguish between different electronic states, or between different structural configurations of the same defect, nor does it indicate how many electronic carriers are involved. Consequently, it is not a useful notation for describing hole defects such as the V_k centre or some vacancy centres with associated charges such as the β centre, and may give a misleading impression if used to describe an H centre as a halide interstitial. Its advantages are most obvious for ionic transport and defect equilibria in non-stoichiometric solids. This scheme uses three superscripts, namely $^{\cdot}$ for the net positive charge, $^{\times}$ for the neutral case and $'$ for a net negative charge; these can be used cumulatively, e.g. $''$ for a doubly negative defect. The site at which the impurity occurs is given by a subscript, where necessary. This use of subscripts is standard in many notations. We now give some examples to compare notations, using the most common of several versions proposed by Kröger and Vink. In our tables later, we shall modify the notation further to avoid other possible sources of confusion.

(a) Vacancy centres in ionic halides and oxides. There is a real problem in that some early papers on oxides labelled the two-electron defect the F centre, whereas other authors called the one-electron defect the F centre. This confusion cannot be ignored. We recommend the use of F^+ for the one-electron defect and of F' or F^0 for the two-electron defect.

Centre	Alkali halides	Alkaline-earth oxides
Anion vacancy		
No carriers	$v_{Cl}^{\bullet}$ α centre or F^+ centre	$v_O^{\bullet\bullet}$ F^{++} centre
One electron	$v_{Cl}^{\times}$ F centre	$v_O^{\bullet}$ F^+ centre
Two electrons	v_{Cl}' F′ centre or F^- centre	$v_O^{\times}$ F^0 or F′ centre
Cation vacancy		
One hole	$V_K^{\times}$ V centre	v_{Mg}' V^- centre
Two hole	V_K' (not seen)	$V_{Mg}^{\times}$ v^0 centre

(b) In GaP the so-called one-electron oxygen centre is $O_P^{\times}$, i.e. the centre one could get (in principle) by removing a P atom and adding an O atom; such operational definitions of charges have a significance lacking in other definitions. The two-electron centre is O_P'.

(c) Transition-metal ions present problems of their own. The commonest system concentrates on the number of 3d electrons, and this can lead to perverse definitions. In ionic crystals, where charges are reasonably well defined (so Mg is 2+ in MgO), one is happy to believe that the 3+ state of Cr in MgO (i.e. $Cr^{\bullet}$ in Kröger–Vink notation), corresponding to the removal of three of the atomic outer electrons (i.e. starting from $3d^5 4s^1$), is $3d^3$. Yet it is not so simple for semiconductors. Here, for various reasons, the neutral impurity ($Cr_{Ga}^{\times}$) is known as the 3+ state, because it has the same number of 3d electrons as does the 3+ state in ionic crystals. There is the interesting corollary that the net *negative centre* (Cr_{Ga}') is described as Cr^{2+}.

Amorphous solids. Here one has to allow for different coordinations and altered topology, as well as different charge states. Thus it may be necessary to assert a particular type of bonding. Whereas for II–VI hosts, like BeO or ZnS, one can start either from an ionic viewpoint (2+ cations and 2− anions) or from a covalent viewpoint (sp hybridisation; see Stoneham (1975) or Catlow and Stoneham (1983)), this flexibility becomes hard to maintain for amorphous solids. First, one adopts a standard coordination (broadly equivalent to a bonding pattern) for each class of atom. Thus there are tetrahedrally bonded species, labelled T (like Si, Ge); there are the pnictides, labelled P (such as N, As, Sb); there are then the doubly bonded species, the chalcogens, labelled C (O, S, Se, Te). For each such species in a 'defect' centre, there is a subscript N, which defines the actual coordination. Secondly, one adopts a reference charge state, and uses a superscript Q to define the charge relative to this reference. So the standard states of the three main types of species are T_4^0 (sp^3 state), P_3^0 (s^2p^3 state) and C_2^0 (s^2p^4 state). The number of 'extra' electrons other than in core states or the N in bonding orbitals is $n = I - Q - N$ for chalcogenides, etc, where $I = 4$ for T species, 5 for P species, and 6 for C species. Thus for Sb ($I = 5$) in α-Si ($N = 4$) the neutral donor defect ($Q = 0$) has $n = 5 - 0 - 4 = 1$ 'extra' electrons and the positive ionised defect has $n = 5 - 1 - 4 = 0$, i.e. no trapped carriers. There is one further convention for antisite defects, i.e. those cases where a chalcogen has chalcogen neighbours, instead of

Table 1. *Systematic of defects in solids.* This table compares defects by type in the best-known crystalline solids. It oversimplifies in several respects, notably by ignoring other crystal structures. Charge states of vacancies are defined by v^{N+}, meaning an ion of charge N- has been removed; for interstitials, i^{M+} means an ion of charge $M+$ is inserted. Traditional labels are given when appropriate.

	Ionic		Covalent		
Type of defect	Alkali halides	Oxides	Other II–VI	III–V	Group IV
Anion vacancy	$v^- = F'$ $v^0 = F$	v^- reported $v^0 = F'$	F', F^+ and 'simple vacancy' reported sometimes associated with impurities	No confirmed reports	Diamond: (v^+), v^0 = GR1, v^- = ND1 Silicon: (v^{2+}), v^+, v^0, v^-, v^{2-} Germanium: v^0, v^-, not v^+(?)
Cation vacancy	$v^0 = V_F$ v^- = simple vacancy	v^0 v^- v^{2-} = simple vacancy	v^0 v^- v^{2-} = simple vacancy	v^0 in GaP	
Polyvacancies	Divacancy; M, R, N centres; colloids	Anion vacancy; aggregates; voids		Possibly colloids	Divacancies in various charge states; chains of vacancies; voids
Interstitials	i^0 = H centre i^+ = simple cation interstitial	O^{2-} in fluorite	Evidence very indirect, although interstitial dislocation loops are easily found		Inferred from reactions under irradiation and from defect aggregates at high temperatures
Other intrinsic defects	Halogen molecule in anion–cation divacancy; self-trapped hole; self-trapped exciton	Vacancy–interstitial complexes; shear planes, small polarons in some systems		Antisite defects	Atoms with non-standard coordination in amorphous material
Important impurities	Molecular ions: OH^-, O_2^-; substitutional Tl, halogen and alkali ions; hydrogen (many forms)	Alkalis (acceptors) and halogens (donors); transition-metal ions (many charge states)		Shallow donors, acceptors and isovalent (e.g. N in GaP) impurities; deep centres (transition metals, Au, etc.); impurities like H or O which were long believed benign (the converse is true, e.g. through the role of H in passivation or of O as thermal-donor precursor)	

those of another species. The convention is to use primes, so a twofold-coordinated chalcogen with one chalcogen neighbour would be C_2', and with two such neighbours C_2''. This should not be confused with Kröger–Vink notation.

3. Organisation of tables

Our plan is to deal with one material (or type of material) at a time, and to cross-reference these where feasible by use of those nomenclatures that are more general (e.g. Kröger–Vink notation). Thus the order we shall use is the following.

Ionic crystals (section 4): most of the information is common to all the ionics, though we shall sometimes need to distinguish between them; in such cases, the order is NaCl-structure halides, fluorite-structure halides, and ionic oxides (usually sixfold-coordinated).
Silica (section 5).
Semiconductors (section 6): tetrahedrally coordinated II–VI compounds, and III–V compounds.
Valence crystals (section 7): diamond, silicon, and germanium.
Special hosts (section 8): amorphous semiconductors, muonium in non-metals, ice, and polyacetylenes.

For each crystal type, we have a further subdivision, namely:

(i) Defects with labels. These may be merely signals, i.e. there may be no confirmed model. We shall give details in the order (a) alphabetical (i.e. a or A before b or B) with Greek separated out, and (b) numerical, e.g. 3H before 3R before 4H.

(ii) Defects with no names, but known merely by their signal, e.g. the centre with $g = 2.343$, etc. These are ordered according to the type of experiment and by the magnitude (so one might have $g = 2.343$ between $g = 2.236$ and $g = 2.453$). In this group, we shall need to distinguish between techniques, but no confusion should arise (optical energies are, of course, not the same as thermal or electrical or deep-level transient spectroscopy levels).

(iii) A partial list of defects that are simply called by what they are, i.e. the model is well established. We have only included cases that we feel are useful in the context of (i) and (ii).

The references for individual tables are given with the tables themselves, since we have found that this is much clearer than a consolidated list. General references and further reading are given at the end of the paper.

4. Ionic crystals

Our lists are for the five main types of crystal, each identified by a specific abbreviation:

AFL Alkali fluorides (these being a subset of AH).
AH Alkali halides.
AHy Alkali hydrides.
AEH Alkaline-earth halides.

O Oxides, principally the sixfold-coordinated oxides like MgO; note that the same defects in fourfold oxides are listed under semiconductors (section 6), and that silica (section 5) and ice (section 8) are listed elsewhere. Most of the oxide centres are given at the end of this section.

In the tables, the column headed 'Model description' indicates which defects are linked to the signal or centre tables for a range of related host crystals. Sometimes it is advantageous to refer to a particular host, and we do this in the second column. Since it is helpful to have specific examples to demonstrate the Kröger–Vink notation, we have chosen KCl and MgO for illustration where this is useful. To avoid confusion later, we shall use systematically the slightly non-standard abbreviations v (vacancy), i (interstitial) and nn (nearest neighbour). In these tables we have also omitted notations that clearly indicate the chemical nature of the defect being studied, e.g. KCl : Na^+ is a Na^+ defect on the K^+ site. The number of such systems is enormous. As a result, some types of defects that have no special labels (such as the off-centre defects Li^+ in KCl and Ag^+ in RbCl) are also excluded.

We give, too, the experimental methods used to observe the defect signals and often used further to identify the signal with a specific model. The abbreviations used in the tables are:

ESR electron spin resonance
ENDOR electron–nuclear double resonance
ODMR optically detected magnetic resonance
FIR far-infrared spectroscopy
MCD magnetic circular dichroism

Other optical methods are written in full.

Signal or centre	Example of Kröger–Vink notation	Host crystals	Model description	Some experimental techniques	Ref.
α	$[v^{\times}_{CL}h^+]$	AH	Excitation of a halogen ion near a halogen-ion vacancy with a transfer of an electron from the halogen to the vacancy to form a (hole–F centre)-like configuration; equivalent to F^+ centre excitation	Optical absorption and luminescence	[1, p 118]
α_A	$[v^{\times}_{CL}Li_K h^+]$	AH	Excitation of a halogen ion next to an impurity alkali–anion vacancy pair to form a (hole–F_A)-like configuration	Optical absorption	[1, p 197]
β		AH	Excitation of a halogen ion near an F centre with a transfer of an electron from the halogen to the F centre to form a (hole–F′)-like configuration	Optical absorption and luminescence	[1, p 93]

Signal or centre	Example of Kröger–Vink notation	Host crystals	Model description	Some experimental techniques	Ref.
β^*		AH	β for F* (excited F centre)	Laser spectroscopy	[1, p 268]
β_A		AH	Excitation of a halogen ion next to an F_A centre with a transfer of an electron from the halogen to the F_A centre to form a (hole–F'_A)-like configuration	Optical absorption	[1, p 197]
A_F		AH	F centre adjacent to a nn metal cation with high ionisation potential (Cu, Ag, Tl, In, etc.); similar to an F_A centre, but electron more localised on the metal ion	ESR	[2]
F	$v_{Cl}^{\times}$	AH AHy	An electron at an anion vacancy in alkali halides (two electrons in an anion vacancy in alkaline-earth halides are sometimes referred to as an F centre; we label it F′)	Optical absorption and emission, ESR, Raman, ENDOR	[1, p 55; 3, p 276]
F_A	$v_{Cl}^{\times}Li_K$	AH	F centre associated with a nn alkali impurity cation, e.g. F_A(Li): F_A(I) centres have emission bands close to the F centre emission band; F_A(II) centres have emission bands well below the F centre emission band	Optical absorption and emission	[1, p 181]
F_B	$v_{Cl}^{\times}Li_KLi_K$	AH	F centre next to two nn alkali impurities	Optical absorption and emission	[6, p 185]
F_H	$v_{Cl}^{\times}Br_{Cl}$	AH	F centre adjacent to a monovalent nn anion impurity (e.g. Br)	Optical and IR absorption	[4, p 343]
$F_Z = Z_1$					
F^*		AH	F centre in relaxed excited state	Optical absorption, ESR	[1, p 270]
F^+		AH	Anion vacancy (ionised F centre); see α centre	Optical absorption	[3, p 280; 5, p 14]
F′	v'_{CL}	AH	Two electrons on an anion site, found in singlet F'_S and triplet F'_T configurations	Optical absorption	[1, p 119]

Signal or centre	Example of Kröger–Vink notation	Host crystals	Model description	Some experimental techniques	Ref.
$F^- = F'$					
F'_A	$v_{Cl}^{\cdot}Li_K$	AH	F' centre adjacent to monovalent nn cation impurity usually an alkali metal, e.g. F'_A(Li)	Optical absorption and emission	[1, p 197]
$F_A^- = F'_A$					
F_2	$(v_{Cl}^{\times})_2$	AH	Two F centres on nn anion sites; NaCl type along ⟨110⟩; CsCl type along ⟨100⟩; found in both singlet and triplet configurations; F_2 = M	Optical absorption and luminescence	[1, p 110; 3, p 281; 5, p 9]
F_2^+	$v_{Cl}^{\times}v_{Cl}^{\bullet}$	AH	Singly ionised F_2 centre (one electron shared in two neighbouring anion vacancies); $F_2^+ = M^+$	Optical absorption, MCD	[3, p 281; 5, p 9]
$(F_2^+)_A$	$v_{Cl}^{\times}v_{Cl}^{\bullet}Li_K$	AH	F_2^+ centre adjacent to alkali defect cation	Optical absorption, IR, laser-active	[4, p 541]
F_2^-	$v_{Cl}^{\times}v'_{Cl}$	AH	Three electrons bound to two ⟨110⟩ neighbouring anion vacancies	Optical absorption and emission, laser-active	[3, p 281; 5, p 9]
$(F_2)_A$	$(v_{Cl}^{\times})_2Li_K$	AH	F_2 centre with a nn impurity alkali ion ($(F_2)_A = M_A$ centre), e.g. $(F_2)_A(Li^+)$	Optical absorption and emission	[6, pp 167, 185]
F_3	$(v_{Cl}^{\times})_3$	AH AEH	Three F centres on nn anion sites in form of an equilateral triangle (F_3 = R)	Optical absorption, luminescence, ESR	[1, p 115; 5, p 11]
F_3^+	$(v_{Cl}^{\times})_2v_{Cl}^{\bullet}$	AH	Singly ionised F_3 centre; two electrons on three nn anion sites	Optical absorption and emission	[5, p 11]
F_3^-	$(v_{Cl}^{\times})_2v'_{Cl}$	AH	One additional electron bound to an F_3 centre	Optical absorption and emission	[5, p 11]
H	$[Cl_2]_{Cl}^{\times}$	AH AEH	⟨110⟩ X_2^- molecular ion on a halogen site (X = halogen), e.g. Br_2^- (⟨111⟩ orientation in LiF); pairs of H centres may contribute to the V bands	Optical, ESR	[1, p 131]
H_A	$[Cl_2]_{Cl}^{\times}Li_K$	AH	H centre adjacent to nn alkali impurity cation	Optical absorption, ESR	[1, p 133; 4, p 353]
H_i^-	H'_i	AH	Interstitial negative hydrogen ion ($H_i^- = U_1$)	Optical absorption, FIR gap mode	[1, p 123]

Signal or centre	Example of Kröger–Vink notation	Host crystals	Model description	Some experimental techniques	Ref.
H_i^0	$H_i^\times$	AH	Interstitial hydrogen atom at a point of T_d symmetry in the lattice ($H_i^0 = U_2$)	Optical absorption	[1, p 123; 6, p 81]
$H_i^0(Y^-)$	$H_i^\times Br_{Cl}^\times$	AH	Perturbed H_i^0 centre with one of nn halogens replaced by an impurity halogen Y^-	Optical absorption, ESR, luminescence, Raman	[6, p 81]
H_s^0	$H_{Cl}^\bullet$	AH AEH	Substitutional hydrogen atom on anion site ($H_s^0 = U_3$)	IR absorption	[5, p 20]
H_s^-	$H_{Cl}^\times$	AH AEH	H^- or D^- ion at a halogen site ($H_s^- = U$ centre)	Optical absorption, no luminescence, FIR local mode	[1, p 123]
H_V	$[Cl_2]_{Cl}^\times v_K'$	AH	H centre adjacent to a cation vacancy	ESR (not clearly observed)	[7, p 371]
H^-H^-	$(H_{Cl}^\times)_2$	AH	Pair of H_s^- centres on nn anion sites	IR local mode	[5, p 58]
$I = X_i^-$					
IV dipole		AH	Impurity–vacancy dipole; divalent cation impurity adjacent to a cation vacancy	Optical absorption, luminescence, ionic thermal currents	[4, p 66]
K		AH	Higher excited-state absorption band of F centre	Optical absorption, ESR	[3, p 277; 8, p 238]
L_1, L_2, L_3		AH	Higher excited-state absorption bands of F centre, above K band	Optical absorption	[3, p 277; 8, p 238]
$M = F_2$					
$M_A = (F_2)_A$					
Muonium		AH AEH Oxides	Positive muon plus electron	Muon spin resonance	[12]
$(M^{3+} + e)$		AEH	Electron bound to a trivalent impurity ion M^{3+} to form shallow hydrogenic atom	Optical absorption	[6, p 139]
N	$(v_{Cl}^\times)_4$	AH	Four F centres(?) or three F centres in different arrangement from R?	Optical absorption	[1, p 117]
N_1	$(v_{Cl}^\times)_4$	AH	Four F centres in a (111) plane?	Optical absorption	[9]

Signal or centre	Example of Kröger–Vink notation	Host crystals	Model description	Some experimental techniques	Ref.
N_2		AH	Proposed model of four F centres in a tetrahedral arrangement, not yet clearly identified	Optical absorption	[9]
$R = F_3$					
$R' = F_3^-$					
$R^+ = F_3^+$					
STE		AH	Self-trapped exciton, usually described as an electron bound to a V_k(hole) centre, i.e. STE=[V_kc]	Optical absorption	[6, p 69]
$U = H_s^-$					
$U_1 = H_i^-$					
$U_2 = H_i^0$					
U_{2x}	$H_i^\times[OH]_{Cl}^\times$	AH	U_2 centre adjacent to OH^- defect	Optical absorption, photodissociation	[6a]
$U_3 = H_s^0$					
V		AH	Cation vacancy with a hole at a nn		[7, p 210]
V^-	v_K'	AH	Cation vacancy		[7, p 210]
V bands		AH	V, V_2, V_3 and V_4 optical bands are associated with molecular halogen ions of the form X_n^-; e.g. linear defect X_3^-		[6, pp 114, 116]
$V_1 = H_A$					
V_4		AH	Possibly a linear molecular halogen ion X_3^- in a cation–anion vacancy	Optical absorption?	[5, p 15]
V_F		AH	A hole centre in which the hole is shared between two nn halogens next to a cation vacancy	Optical absorption	[3, p 289; 5, p 16]
V_k		AH	Self-trapped hole centre, with the hole shared between two neighbouring halogens (an X_2^- or $(XY)^-$-like ion, X, Y halogens); a *small polaron*	Optical absorption, ESR	[1, p 131]
V_{kA}		AH	V_k centre with nn impurity alkali cation	Optical absorption, ESR	[3, p 291]

Signal or centre	Example of Kröger–Vink notation	Host crystals	Model description	Some experimental techniques	Ref.
V_{kAA}		AH	V_k centre with two nn alkali impurity cations	ESR, optical absorption	[3, p 291]
$[V_k e]$ = STE		AH AEH	Self-trapped exciton	ESR optical absorption	[8]
V_t		AFl	Hole localised on three adjacent fluoride ions in a (100) plane	ESR	[3, p 291]
X_2^-		AH	Self-trapped hole; see V_k centre	Optical absorption	[1, p 131; 7, p 211]
XY^-		AH	Hole trapped at a halide impurity; a V_k-like centre	Optical absorption	[1, p 131; 7, p 211]
X_i^-	Br_i'	AH	Interstitial halide ion X^- probably at a point of T_d symmetry (I centre)	Inferred from other measurements; no direct observation	[5, p 14]
X_3^-		AH	Linear molecular ion of halogens; axis may be along ⟨100⟩, ⟨110⟩ or ⟨111⟩; likely to correspond to V_2, V_3 or V_4 absorption bands	Optical absorption	[6, pp 114, 116, 271]
X_n^-		AH	Polyhalide; contributes to part of V_2 band	Optical absorption	[6, pp 114, 116, 271]
Z_1	$v_{Cl}^{\times}M_K^{\bullet}v_K'$	AH	F centre adjacent to an impurity–vacancy (IV) dipole formed by a divalent cation defect and cation vacancy	Optical absorption	[5, p 20]
Z_2	$v_{CL}'M_K^{\bullet}$	AH	Divalent impurity cation plus two electrons in a nn anion vacancy (M^{2+} and F′ centre)	Optical absorption	[6, p 237]
Z_2^+	$v_{CL}^{\times}M_K^{\bullet}$	AH	F centre with nn divalent cation; singly ionised Z_2 centre	Magneto-optical, laser-active, optical absorption	[6, p 89]
Z_4		AH	Divalent cation with nn F_2 centre?	Optical absorption	[6, p 167]
Oxides					
F′ or F^0	$v_O^{\times}$	O	Two electrons in an oxygen vacancy; similar to the F′ centre in the alkali halides; sometimes referred as an F centre	Optical	[8, p 240]
F^+	$v_O^{\bullet}$	O	One electron in an oxygen vacancy; similar to the F centre in the alkali halides	ESR	[8, p 240]

Signal or centre	Example of Kröger–Vink notation	Host crystals	Model description	Some experimental techniques	Ref.
F_c^+		O	An electron bound to adjacent cation and anion vacancies; i.e. an F^+ centre with an adjacent cation vacancy	ESR	[10, p 811]
F_t	$v_O^{\bullet} v_{Mg}'' v_O^{\bullet}$	O	Two nn F^+ centres along a (100) direction with a cation vacancy between them	ESR	[10, p 627]
$P = F_c^+$		O	Electron trapped at anion–cation vacancy pair		
V^-	v_{Mg}'	O	Positive hole trapped at a divalent cation vacancy	ESR	[11, p 225]
V_F	$v_{Mg}' F_O^{\bullet}$	O	A linear defect consisting of a hole on an oxygen site, a divalent cation vacancy and an F^- ion	Optical	[11, p 233]
V_M or V_{Al}	$v_{Mg}' Al_{Mg}^{\bullet}$		A V^- centre with a trivalent $M^{3+}(Al^{3+})$ ion in the next nn position to the cation vacancy; sometimes also used to specify a metal ion vacancy	ESR, ENDOR	[11, p 229]
V^0		O	Two holes trapped on different oxygen atoms, adjacent to a divalent cation vacancy	ESR, optical	[10, p 629; 11, p 225]
V_{OH}		O	A linear defect consisting of a hole on an oxygen site, a divalent cation vacancy and OH^- ion; similar to V_F	Optical, IR	[11, p 233]

[1] Fowler W B 1968 *Physics of Color Centers* (New York: Academic)
[2] Baranov P G 1983 *Sov. Phys.–Solid State* **25** 507
[3] Watts R K 1977 *Point Defects in Crystals* (New York: Wiley)
[4] 1985 *Cryst. Latt. Defects Amorph. Mater.* **12**
[4a] 1989 *Cryst. Latt. Defects Amorph. Mater.* **18**
[5] Farge Y and Fontana M P 1979 *Electronic and Vibrational Properties of Point Defects in Ionic Crystals* (*Defects in Crystalline Solids 11*) (Amsterdam: North-Holland)
[6] 1983 *Lattice Defects in Ionic Crystals* (*Dublin*, 1982): *Radiat. Eff.* **72**
[6a] 1983 *Lattice Defects in Ionic Crystals* (*Dublin*, 1982); *Radiat. Eff.* **73**
[7] Crawford J and Slifkin L 1972 *Point Defects in Solids* vol 1 (New York: Plenum)
[8] Hayes W and Stoneham A M 1985 *Defects and Defect Processes in Nonmetallic Solids* (New York: Wiley)
[9] Pick H 1960 *Z. Phys.* **159** 69
[10] Stoneham A M 1975 *Theory of Defects in Solids* (Oxford: Oxford University Press)
[11] Seltzer M S and Jaffee R I (ed) 1974 *Defects and Transport in Oxides* (New York: Plenum)
[12] Cox S F J 1987 *J. Phys. C: Solid State Phys.* **20** 3187

5. Silica and similar oxides

We list here defect labels for both quartz and vitreous silica. No doubt similar forms occur in other structures of silica, and indeed the extent to which defects depend on the host structure is important in defining models. Oxides similar in some respects will be GeO_2, SnO_2, possibly TeO_2 and (in a more limited sense) H_2O. Since some of the links between optical and spin resonance data are in doubt, we have divided the lists up by technique. Thus the E_1' centre appears in both sections 5.1 and 5.2. The several experimental methods are these:

ESR	electron spin resonance
ODMR	optically detected magnetic resonance
PL	photoluminescence
IR	infrared absorption
DLTS	deep-level transient spectroscopy

5.1. Quartz: optical data

Defect label	Model/technique	Ref.
7.8 eV	Optical absorption	[1]
6.7 eV	Optical emission	[1]
5.85 eV	E_1' absorption	[1]
5.2 eV	E_2' absorption	[1]
5 eV	B_2 absorption band	[1]
4.43 eV	Ge(A), Ge(C) absorption	[1]
4.3 eV	Optical emission associated with oxygen deficiency	[1]
2.9 eV	'Smoky' quartz; absorption associated with Al causes hole to hop from one oxygen to another	[1, 2]
2.8 eV	Intrinsic luminescence of self-trapped exciton excited > 9 eV	[3]
2.5 eV	Extrinsic luminescence	[3]

[1] Griscom D L 1979 *Proc. 33rd Frequency Control Symp.* (Washington DC: Electronic Industries Association)
[2] Schirmer O F 1976 *Solid State Commun.* **18** 1349
[3] Itoh C, Tanimura K, Itoh N and Itoh M 1989 *Phys. Rev.* B **39** 11133

5.2. Quartz

Defect label	Model	Technique	Ref.
Spin resonance data			
E_1'	Asymmetrically relaxed, positive oxygen vacancy, V_O^+; electron on the short-bond Si	$\equiv Si^+ \ {}^0S \equiv$ ESR	[1–3]
E_4'	Off-centre substitutional H_O; electron on the long-bond Si	$\equiv Si^0$ HSi $\equiv$ ESR	[3]

Defect label	Model	Technique	Ref.
E_2'	Inverted form of E_4'	$\equiv Si^0\ HSi \equiv$ ESR	[4]
$Ge(E_1')$	Ge variant of E_1'	$\equiv Si^+\ ^0Ge \equiv$ ESR	[3]
$Ge(E_2')$	Ge variant of E_2'	$\equiv Ge^0\ ^+Ge \equiv$ ESR	
$(GeO_4)^-$	Electron trapped by substitutional Ge_{Si}^0 site	ESR	[1, 3, 5]
$(GeO_4^-, M^+)^0$	Alkali-ion compensated Ge_{Si}^- centre		[3]
$(PO_4)^0$	Electron trapped by substitutional P_{Si}^+ site (P_2 centre)	ESR	[6]
$(AlO_4)^0$	Hole trapped on pp orbital on nn oxygen adjacent to substitutional Al_{Si}^- site; hole can hop between oxygens; Al^0	ESR	[1, 3]
$(AlO_4, M^+)^0$	Diamagnetic precursor of above, alkali compensation		[1, 3]
$(BO_4)^0$	Boron analogue of $(AlO_4)^0$	ESR	[1]
$[(HO)_4]^+$	Four hydrogens substituting for one Si, with hole trapped on oxygen pp state, as in Al^0	ESR	[3]
$[H_3O_4]^+$	Three hydrogens substituting for Si, with unpaired electron on remaining oxygen dangling bond	ESR	[3]
H^0	Atomic hydrogen in interstice	ESR	[3]
BR	Unmodelled centre, perhaps involving O–O bond	ESR	[7]
β	Na_n, Ge trapped electron centres	ESR	[1]
H(I)	Oxygen π hole near Ge_{Si}	ESR	[8]
E_3'	H-related centre	ESR	[9]
Optical data			
STE	Self-trapped exciton; $S = 1$; see 2.8 eV luminescence	ODMR	[10]

[1] Griscom D L 1978 *Physics of SiO₂ and its Interfaces* ed S T Pantelides (Oxford: Pergamon)
[2] Griscom D L 1979 *Proc. 33rd Frequency Control Symp.* (Washington DC: Electronic Industries Association)
[3] Weil J A 1984 *Phys. Chem. Min.* **10** 149
[4] Fiegl F 1985 *Phys. Rev. Lett.* **55** 2614
[5] Isoya J, Weil J A and Claridge R 1978 *J. Chem. Phys.* **69** 4876
[6] Uchida Y, Isoya J and Weil J A 1979 *J. Phys. Chem.* **83** 3462
[7] Baker J M and Robinson P T 1983 *Solid State Commun.* **48** 551
[8] Hayes W and Jenkin T 1986 *J. Phys. C: Solid State Phys.* **19** 6211
[9] Maschmeyer D and Lehmann G 1984 *Solid State Commun.* **50** 1015
[10] Hayes W, Kane M J, Salminen O, Wood R L and Doherty S P 1984 *J. Phys. C: Solid State Phys.* **17** 2943

5.3. *Amorphous silica*

Defect	Model	Technique	Ref.
STH1	Self-trapped hole on 1 bridging oxygen		[14]
STH2	Self-trapped hole on 2 bridging oxygens		[14]
E′	Generic Si dangling-bond centre	ESR	[2]

Defect	Model	Technique	Ref.
E'_g	Neutron or gamma-ray-induced centre; most similar to V_O^+	ESR	[2]
E'_b	X-irradiation, axially symmetric, ≡Si centre	ESR	[2]
E'_a	Radiolytic centre induced by x-rays	ESR	[2]
$-O°$	Non-bridging oxygen (NBO) hole centre; loosely associated proton; 'wet oxygen hole centre' ('wet OHC')	ESR	[2]
$-O-O°$	Superoxy (peroxy) radical; 'dry OHC'		[2]
N	$(NSi_2)^+$ centre	ESR	[3]
N′	$(NSi_4)^0$, trigonally distorted as in Si		[15]
$(AlO_4)^0$	Al centre	ESR	[4]
$(BO_4)^0$	B centre	ESR	[5]
$(AlO_3)^-$	Al variant of E′; trivalent Al; trapped electron	ESR	[6]
P_1	E′ analogue of P, ≡ P	ESR	[7]
P_2	Four-coordinated P	ESR	[7]
P_4	Hole on $=P^0$	ESR	[7]
POHC	Hole trapped between two oxygens, in $=P=O_2$ group	ESR	[7]
Optical data (for a survey, see [8])			
7.6 eV	Superoxy radical; E band	Absorption	[2]
7.6 eV	Oxygen deficiency band		[9]
7.2 eV	D band; after heavy-ion irradiation	Absorption	[2]
5.8 eV	E′ centre; oxygen vacancy; various related centres are noted	Absorption	[2]
5.0 eV	B_2 band; debated origin; oxygen vacancy?	Absorption	[2, 9]
4.8 eV	Non-bridging oxygen?	Absorption	PL [2, 10]
4.3 eV	5.0, 7.6 eV excitation; debated origin	Emission	[2]
2.8 eV	Self-trapped exciton, as in quartz	Emission	[11]
2.65 eV	5.0 eV excitation	Emission	[9]
2.0–2.6 eV	Holes on non-bridging oxygens	Absorption	[9]
1.9 eV	Seen in drawn fibres	Absorption	[2]
1.9 eV	Non-bridging oxygen	Absorption	[10, 12]
1.9 eV	Non-bridging oxygen	Emission	[10, 12]
2.75 μm	O–H group vibration	IR absorption	

[1] Weil J A 1984 *Phys. Chem. Mineral.* **10** 149
[2] Griscom D L 1985 *J. Non-Cryst. Solids* **73** 51
[3] Friebele E J, Griscom D L and Hickmott T W 1985 *J. Non-Cryst. Solids* **71** 351
[4] Uchida Y, Isoya J and Weil J A 1979 *J. Phys. Chem.* **83** 3462
[5] Griscom D L, Sigel G H and Ginther R J 1976 *J. Appl. Phys.* **47** 960

[6] Brower K L 1979 *Phys. Rev.* B **20** 1799
[7] Griscom D L, Friebele E J, Long K L and Fleming J W 1983 *J. Appl. Phys.* **54** 3743
[8] Weber M (ed) 1985 *CRC Laser Handbook* (Boca Raton, FL: CRC Press) p 381 et seq
[9] Tohman R *et al* 1989 *Phys. Rev.* B **39** 1337
[10] Tohman R *et al* 1989 *Appl. Phys. Lett.* **54** 1650
[11] Itoh C, Tanimura K, Itoh N and Itoh M 1989 *Phys. Rev.* B **39** 11183
[12] Devine R, Fiori C and Robertson J 1986 *Mater. Res. Soc. Symp. Proc.* **61** 177
[13] Bell T, Hetherington G and Jack K H 1962 *Phys. Chem. Glasses* **3** 141
[14] Griscom D L 1989 *Phys. Rev.* B **40** 4224
[15] Tsai T E, Griscom D L and Friebele E J 1988 *Phys. Rev.* B **38** 2140

5.4. The SiO_2:Si interface (thermally grown silicon dioxide on crystalline silicon)

Defect	Electrical level (V)	Model	Technique	Ref.
P_b	$E(-/0)$ cb − 0.2	≡ Si site on Si side of interface	ESR	[1]
	$E(0/+)$ cb − 0.8	$g/2.0055$, $U/0.6$ eV	DLTS	[2]
Q_f		Fixed charge in oxide		[3, 4]
Q_n		Mobile charge in oxide		[3, 4]
Q_{it}		Interface fixed charge (e.g. P_b) ('fast' states)		[3, 4]
Q_{Ot}		Oxide trapped charge ('slow' states)		[3, 4]
ND		'New donors' in silicon after thermal treatment at 650–800 °C, and apparently associated with SiO_x precipitates (a) as interface states and (b) bound by the net precipitate charge		[5]

[1] Poindexter E H, Caplan P J, Deal B E and Razouk R R 1981 *J. Appl. Phys.* **52** 879
[2] Poindexter E H, Gerardi G J, Ruckel M E, Caplan P J, Johnson N M and Biegelsen D K 1985 *J. Appl. Phys.* **56** 2844
[3] Deal B E 1980 *IEEE Trans Electron. Devices* **ED-27** 606
[4] Griscom D L 1985 *J. Appl. Phys.* **58** 2524
[5] Pensl G, Schulz M, Hölzlein K, Bergholz W and Hutchinson J L 1989 *Appl. Phys.* A **48** 49

5.5 SnO_2

Defect	Electrical level (V)	Model	Technique	Ref.
v_O	$E(0/+)$ cb − 0.035	Shallow double donor	PL	[1]
F_O	$E(0/+)$ cb − 0.034	Shallow donor	PL	[1]
Sb_{Sn}	$E(0/+)$ cb − 0.035	Shallow donor	PL	[1]
Al_{Sn}		Hole trapped in oxygen pp orbital adjacent to Al_{Sn} site or to another group III ion (Ga, In) on the Sn site		[2]

[1] Agekyan V T 1977 *Phys. Status Solidi* a **43** 11
[2] Zwingel D 1976 *Phys. Status Solidi* b **77** 171

6. Compound semiconductors

These systems have defect centres whose features have much in common with ionic crystals and with valence crystals; indeed, it can be a matter of convention as to the way the electronic structure is described.

Apart from the standard notation, we shall use JT to identify defects with reduced symmetry attributed to the Jahn–Teller effect.

6.1. II–VI compounds and PbTe

6.1.1. ZnO

Defect	Electrical level (V)	Model	Technique	Ref.[a]
$v_O(F^+)$		Oxygen vacancy; similar to F^+ centre in alkaline-earth oxides		[1; 2, p 249]
$v_{Zn}(V^-)$		Zn vacancy; JT distorted		[1; 2, p 249]
Li_{Zn}		Deep acceptor		[2, p 243]
Na_{Zn}				[2, p 243]
Li_i		Interstitial donor		[2, p 243]

[a] References at end of section 6.1.9.

6.1.2. ZnS

Defect label	Electrical level (V)	Model	Technique	Ref.[a]
$v_S(F^+, F^0)$	(+/0)	S vacancy	ESR	[1; 2, p 249]
$v_{Zn}(V^-)$	$E(2-/-)$ $\sim$ vb + 1.1	Zn vacancy; JT distorted; v^- is C_{3v} so spin on one sulphur	ESR, ODMR	[1, 3]
F_S		Substitutional donor, deep	PL	[2, 4]
Cl_S		Substitutional donor, deep	PL	[2, 4]
Br_S		Substitutional donor, deep	PL	[2, 4]
I_S		Substitutional donor, deep	PL	[2, 4]
Te_S	$E(0/+)$ vb + 0.44	Isoelectronic donor	PL	[5]
P_S	(−/0)	Deep acceptors (JT)		[5]
As_S	(−/0)	Deep acceptor (JT)		[5]
Sb_S	(−/0)	Deep acceptor (JT)		[5]

Defect label	Electrical level (V)	Model	Technique	Ref.[a]
Al_{Zn}	(0/+)	Shallow donor		[2, p 249; 4]
Ga_{Zn}	(0/+)	Deep donor		
In_{Zn}	(0/+)	Deep donor		
Li_{Zn}		Acceptor		
A		A centre acceptor; v_{Zn}–donor complexes; produces self-activated (SA) luminescence (~4700 Å)	PL, ESR, ODMR	[2, p 252; 4]
M		Nn v_S–v_S pair		

[a] References at end of section 6.1.9.

6.1.3. ZnSe

Defect label	Electrical level (V)	Model	Technique	Ref.[a]
v_{Se}	$E(0/+)$ cb − 0.02 $E(+/2+)$ cb − 0.3	Se vacancy		[1, 6]
v_{Zn}	(−/2/) mid-gap	Zn vacancy; JT distorted	ODMR, ESR	[1, 7]
Zn_i		Zn^+ interstitial		[7a]
$v_{Zn}Zn_i$		v_{Zn}^-, Zn_i^{2+} Frenkel pair		[7b]
F_{Se}	$E(0/+)$ cb − 0.029	Se-site donor	PL	[2, p 240]
Cl_{Se}	$E(0/+)$ cb − 0.027	Se-site donor	PL	[2, p 240]
Al_{Zn}	$E(0/+)$ cb − 0.026	Zn-site donor		[2, p 240]
Ga_{Zn}	$E(0/+)$ cb − 0.028	Zn-site donor		[2, p 240]
In_{Zn}	$E(0/+)$ cb − 0.029	Zn-site donor		[2, p 240]
Li_i	$E(0/+)$ cb − 0.028	Interstitial donor		[2, p 240]
Na_i	$E(0/+)$ cb − 0.028	Interstitial donor		[2, p 240]
Li_{Zn}	$E(-/0)$ vb + 0.114	Zn-site acceptor		[2, p 240]
Na_{Zn}	$E(-/0)$ vb + 0.128	Zn site acceptor		[2, p 240]
Li_i–Li_{Zn}	—	Self-compensating centres (also Na equivalents)		[8]
P_{Se}	$E(-/0) \sim$ vb + 1	Deep, Se-site acceptor; JT distorted		[2, p 240]
As_{Se}	$E(-/0) \sim$ vb + 1	Deep, JT distorted, Se-site acceptor		[2, p 240]
N_{Se}	$E(-/0)$ vb − 0.085	Shallow acceptor		[5, 9]

Defect label	Electrical level (V)	Model	Technique	Ref.[a]
A		Acceptor; nn v_{Zn}–D_{Se} or 2nn v_{Zn}–D_{Zn} complex (D = donor); causes self-activated luminescence (~6250 Å)		
Pb_{Zn}		Deep double acceptor	ESR	[2]
Ge_{Zn}		Deep double acceptor		[2]

[a] References at end of section 6.1.9.

6.1.4. ZnTe

Defect label	Electrical level (V)	Model	Technique	Ref.[a]
v_{Te}		Te vacancy		[1]
v_{Zn}		Zn vacancy		[1]
D	$E(0/+)$ cb − 0.0183	Shallow donor	PL	[2, 5, 10]
Li_{Zn}	$E(-/0)$ vb + 0.060	Acceptor	PL	[2, 5, 10]
Cu_{Zn}	$E(-/0)$ vb + 0.148	Acceptor	PL	[2, 5, 10]
Ag_{Zn}	$E(-/0)$ vb + 0.121	Acceptor	PL	[2, 5, 10]
P_{Te}	$E(-/0)$ vb + 0.0635	Acceptor	PL	[2, 5, 10]
As_{Te}	$E(-/0)$ vb + 0.079	Acceptor	PL	[2, 5, 10]
O_{Te}	$E(0/+)$ cb − 0.4	Isoelectronic acceptor	PL	[2]

[a] References at end of section 6.1.9.

6.1.5. CdS

Defect label	Electrical level (V)	Model	Technique	Ref.[a]
v_S		Vacancy		[1]
v_{Cd}		Vacancy		[1]
F_S	$E(0/+)$ cb − 0.0351	S-site donor	PL	[2, p 240]
Cl_S	$E(0/+)$ cb − 0.0327	S-site donor		
Br_S	$E(0/+)$ cb − 0.0325	S-site donor		
I_S	$E(0/+)$ cb − 0.0321	S-site donor		
Ga_{Cd}	$E(0/+)$ cb − 0.0331	Cd-site donor		
In_{Cd}	$E(0/+)$ cb − 0.0338	Cd-site donor		
Li_i	$E(0/+)$ cb − 0.0286	Interstitial donor		
Na_i	$E(0/+)$ cb − 0.0315	Interstitial donor		
Li_{Cd}	$E(-/0)$ vb + 0.165	Cd-site acceptor		

Defect label	Electrical level (V)	Model	Technique	Ref.[a]
Na_{Cd}	$E(-/0)$ vb + 0.169	Cd-site acceptor		
P_S	$E(-/0) \sim$ vb + 1	S-site deep acceptor		
As_S	$E(-/0) \sim$ vb + 1	S-site deep acceptor		
Te_S	$E(0/+)$ vb + 0.25	Isoelectronic acceptor		[2, p 255]
A		v_{Cd}–donor complex; cause of self-activated luminescence		

[a] References at end of section 6.1.9.

6.1.6. CdSe

Defect label	Electrical level (V)	Model	Technique	Ref.[a]
v_{Se}		Vacancy		[1]
v_{Cd}		Vacancy		[1]
D	$E(0/+)$ cb − 0.0195	Unknown donor		[2]
Li_{Cd}	$E(-/0)$ vb + 0.109	Cd-site acceptor		[2]
Na_{Cd}	$E(-/0)$ vb + 0.109	Cd-site acceptor		[2]

[a] References at end of section 6.1.9.

6.1.7. CdTe

Defect label	Electrical level (V)	Model	Technique	Ref.[a]
v_{Te}		Vacancy		[1]
v_{Cd}		Vacancy		
Al_{Cd}	$E(0/+)$ cb − 0.014	Cd-site donor		[2, p 240]
In_{Cd}	$E(0/+)$ cb − 0.014	Cd-site donor		[2, p 240]
Li_{Cd}	$E(-/0)$ vb + 0.458	Cd-site acceptor		[11]
Na_{Cd}	$E(-/0)$ vb + 0.059	Cd-site acceptor		[11]
Cu_{Cd}	$E(-/0)$ vb + 0.146			[11]
Ag_{Cd}	$E(-/0)$ vb + 0.107			[11]
Au_{Cd}	$E(-/0)$ vb + 0.263			[11]
N_{Te}	$E(-/0)$ vb + 0.056			[11]
P_{Te}	$E(-/0)$ vb + 0.068			[11]
As_{Te}	$E(-/0)$ vb + 0.092			[11]
Cl_{Te}	$E(-/0)$ cb − 0.014	Te-site donor with some D_x character		[12]

[a] References at end of section 6.1.9.

6.1.8. $Hg_xCd_{1-x}Te$

Defect label	Electrical level (V)	Model	Technique	Ref.[a]
v_{Hg}	$E(-/0) \sim vb + 0.013$	Vacancy, double acceptor	Hall effect	[11]
Al_{Te}	(0/+)	Shallow donor		[11]
In_{Te}	(0/+)	Shallow donor		
Ag	$E(-/0) \sim vb + 0.005$	Metal-site acceptor		[13]
As_{Te}	$E(-/0) \sim vb + 0.005$	Te-site acceptor		
Sb_{Te}	$E(-/0) \sim vb + 0.005$	Te-site acceptor		
O	(0/+)	Donor, unknown configuration		[14]
$0.4E_g$		Defect whose energy level lies at ~0.4 of the gap above vb; v_{Hg}-related	DLTS	[11, 15]
$0.7E_g$		Defect of unknown origin whose energy level lies at ~0.7 of the gap above vb	DLTS	[11, 15]

[a] References at end of section 6.1.9.

6.1.9. PbTe

Defect label	Electrical level (V)	Model	Technique	Ref.
v_{Te}	$(0/+) \sim cb$	Double donor, shallow		[16]
v_{Pb}	$(-/0) \sim vb$	Double acceptor, shallow		[16]
In	$(0/+) \sim cb$	Donor; A1 and T1 are similar		[17]
(No label)	(+/3+) cb	Self-compensation by disproportionation, i.e. the 2+ state forms 1+ and 3+ exothermically		[17]

[1] Watkins G D 1977 *Radiation Effects in Semiconductors* 1976 (*Inst. Phys. Conf. Ser.* 31) ed N B Urli and J W Corbett (Bristol: Institute of Physics) p 95
[2] Watts R K 1977 *Point Defects in Crystals* (New York: Wiley)
[3] Lee K M, O'Donnell K P and Watkins G D 1982 *Solid State Commun.* **41** 881
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[5] Kobayashi A, Sankey O F and Dow J D 1983 *Phys. Rev.* B **28** 946
[6] Shirakawa Y and Kukimoto H 1960 *Solid State Commun.* **34** 359
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[7a] Rong F and Watkins G D 1987 *Phys. Rev. Lett.* **58** 1486
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[10] Venghaus H and Dean P J 1980 *Phys. Rev.* B **21** 1596
[11] Jones C E, James K and Merz J 1985 *J. Vac. Sci. Technol.* A **3** 131

[12] Legros R, Marfaing Y and Triboulet R 1983 *J. Phys. Chem. Solids* **39** 179
[13] Capper P, Gosney J J, Jones C L and Roberts J A 1985 *J. Crystal Growth* **71** 57
[14] Yoshikawa M, Ueda S, Maruyana K and Takigawa H 1985 *J. Vac. Sci. Technol.* A **3** 153
[15] Kobayashi A, Sankey O F and Dow J D 1982 *Phys. Rev.* B **25** 6367
[16] Bauer G, Burkhard H, Heinrich H and Otero A L 1976 *J. Appl. Phys.* **47** 1721
[17] Watkins G D 1984 *Festkorperprobleme* **24** 163

6.2. III–V compounds

6.2.1. GaP

Defect label	Electrical level (V)	Model	Technique	Ref.
P_{Ga}	(0/+)? $E(+/2+)$ cb − 1.1	P-antisite defect	ESR	[1, 2]
v_P	$E(-/0)$ vb + 0.9?	P vacancy, $S = 3/2$; here Hunds' rule dominates over Jahn–Teller	ESR	[3]
	$E(2-/-)$ vb + 0.64			
S	$E(0/+)$ cb − 0.1042	P-site donor		[4]
Se	$E(0/+)$ cb − 0.1026	P-site donor		[4]
Te	$E(0/+)$ cb − 0.0898	P-site donor		
O	$E(0/+)$ cb − 0.896	P-site amphoteric deep trap; 'one-electron centre'	PL	[5]
	$E(-/0)$ cb − 2.03/vb + 1.81	Metastable (0/−) state with strong electron–lattice coupling; 'two-electron centre'		
Si	$E(0/+)$ cb − 0.0825	Ga-site donor	PL	[4]
Ge	$E(0/+)$ cb − 0.2015	Ga-site donor		
Sn	$E(0/+)$ cb − 0.0655	Ga-site donor		[4]
C	$E(-/0)$ vb + 0.0464	P-site acceptor	PL	[6, p 217]
Si	$E(-/0)$ vb + 0.202	P-site acceptor		
Ge	$E(-/0)$ vb + 0.257	P-site acceptor		
Be	$E(-/0)$ vb + 0.0487	Ga-site acceptor	PL	[6, p 217]
Mg	$E(-/0)$ vb + 0.052	Ga-site acceptor		
Zn	$E(-/0)$ vb + 0.0617	Ga-site acceptor		
Cd	$E(-/0)$ vb + 0.0943	Ga-site acceptor		
Bi	$E(0/+)$ vb + 0.040	P-site isoelectronic donor		
N	(−/0) cb	P-site isoelectronic acceptor; only the related exciton (N_x) is bound in GaP ($E_b = 11$ meV) but the (−/0) level is deep in $GaAs_xP_{1-x}$	PL	[6, p 213; 7]

Defect label	Electrical level (V)	Model	Technique	Ref.
S–Si		S_P–Si_P pair; example of type I donor–acceptor pair (same site)	PL	[6, p 213; 7]
Cd–O		Cd_{Ga}–O_P pair; example of type II donor-acceptor pair (opposite site)		[6, p 213; 7]
B–N		$B_{Ga}N_p$; example of isoelectronic donor–acceptor pair	PL	[7]
Li(I)	$E(0/+)$ cb − 0.086	Li_i, Ga neighbours, donor		[6, p 227]
Li(II)	$E(-/0)$ vb − 0.056	Li_i, P neighbours, acceptor		[6, p 227]
V	$E(-/0)$ vb + 0.85	Ga-site substitutional transition-metal ions. See section 2 for charge-state conventions	DLTS	[1,8]
Cr	$E(2-/1)$ vb + 1.5 $E(-/0)$ vb + 1.1 $E(0/+)$ vb + 0.52			
Mn	$E(-/0)$ vb + 0.4			
Fe	$E(-/0)$ vb + 0.7			
Co	$E(-/0)$ vb + 0.4			
Ni	$E(-/0)$ vb + 0.5 $E(2-/-)$ vb + 1.55			
Cu	$E(-/0)$ vb + 0.72 $E(0/+)$ vb + 0.45	Ga-site substitutional transition-metal ions. See section 2 for charge-state conventions	DLTS	[1, 8]
E_1	cb − 1.14	Irradiation-induced electron traps	DLTS	[9, 10]
E_2	cb − 0.23			
E_3	cb − 0.32			
E_4	cb − 0.48			
E_5	cb − 0.62			
E_6	cb − 0.74			

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6.2.2. *GaAs*

Defect label	Electrical level (V)	Model	Technique	Ref.
As_{Ga}		As antisite	ESR	[1]
EL2	$E(0/+)$ vb + 0.75	As_{Ga}-related centre, As_{Ga}–As_i or $As_{Ga} \rightleftharpoons v_{Ga} - A_{Si}$	ESR, DLTS	[2–4]
	$E(+/2+)$ vb + 0.52			[3]
		1.18 eV optical transition to metastable state; this defect provides compensation	ENDOR	[2]
v_{As}		As vacancy; donor		[4]
v_{Ga}		Ga vacancy; acceptor		[4]
As_i		Interstitial; donor		[4]
Ga_i		Interstitial; donor		[4]
Irradiation-induced defects, E_1–H_3 (E for electron traps, H for hole traps)			DLTS	[7, 8]
E_1	cb − 0.045	$v^2 - As$		[7, 8]
E_2	cb − 0.14	$v^- As$		[7, 8]
E_3	cb − 0.30	As sublattice defect		[7, 8]
E_4	cb − 0.76			[7, 8]
E_5	cb − 0.96			[7, 8]
P_1	cb − 0.36			[7, 8]
P_2	cb − 0.50			[7, 8]
P_3	cb − 0.70			[7, 8]
H_0	vb + 0.6			[7, 8]
H_1	vb + 0.29			[7, 8]
H_2 = A	$E(-/0)$ vb + 0.41			[7–9]
H_3 = B	$E(2-/-)$ vb + 0.71	Ga_{As} antisite?		[7–9]
B–As_i		Boron–As interstitial complex	IR	[10]
C–As_i		Carbon–As interstitial complex	IR	[10]
Si_{Ga}	(0/+) cb − 0.00584	Ga-site donor		[11, p 224]
Ge_{Ga}	(0/+) cb − 0.06608	Ga-site donor		
Sn_{Ga}	$E(0/+)$ cb − 0.006	Ga-site donor		
S_{As}	$E(0/+)$ cb − 0.0061	As-site donor		
Se_{As}	$E(0/+)$ cb − 0.00589	As-site donor		
Te_{As}	$E(0/+)$ cb − 0.006	As-site donor		
O_{As}	$E(0/+)$ cb − 0.75	As-site donor		

Defect label	Electrical level (V)	Model	Technique	Ref.
Li	$E(0/+)$ cb − 0.006	Interstitial donor		
Be_{Ga}	$E(-/0)$ vb + 0.03	Ga-site acceptor		[11, p 224]
Mg_{Ga}	$E(-/0)$ vb − 0.03	Ga-site acceptor		
Zn_{Ga}	$E(-/0)$ vb + 0.0314	Ga-site acceptor		
Cd_{Ga}	$E(-/0)$ vb + 0.0354	Ga-site acceptor		
C_{As}	$E(-/0)$ vb + 0.0267	As-site acceptor		
Si_{As}	$E(-/0)$ vb + 0.0352	As-site acceptor		
Ge_{As}	$E(-/0)$ vb + 0.0412	As-site acceptor		
Sn_{As}	$E(-/0)$ vb + 0.171	As-site acceptor		
N_{As}	$E(-/0)$	Isoelectronic acceptor; conduction band resonance in GaAs, but deep trap in $Ga_xAl_{1-x}As$ alloys	PL	[10]
DX		Various donor–defect complexes of unknown configuration, with strong electron–lattice coupling in $Al_xGa_{1-x}As$ and $GaAs_xP_{1-x}$ alloys	DLTS	[11–13]
Li	(−/0)	Compensating acceptor, Ga site		[10, p 224]
Ti	$E(0/-)$ vb − 0.98	Transition-metal ions; substitutional at Ga site	ESR, DLTS	[14, 15]
V	$E(0/1)$ vb + 1.3			
Cr	$E(2-/-)$ cb $E(-/0)$ vb + 0.82 $E(0/+)$ vb + 0.45	See section 2 for charge-state conventions		
Mn	$E(-/0)$ vb + 0.1			
Fe	$E(-/0)$ vb + 0.54			
Co	$E(-/0)$ vb + 0.16			
Ni	$E(-/0)$ vb + 0.20 $E(2-/-)$ vb + 1.04			
Cu	$E(-/0)$ vb + 0.45 $E(0/+)$ vb + 0.16			

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6.2.3. InP

Defect label	Electrical level (V)	Model	Technique	Ref.
v_P	$E(0/+)$ cb − 0.99	P vacancy	PL	[1]
v_{In}	$E(0/-)$ vb + 1.21	In vacancy or P interstitial	PL	[1]
P_{In}	1.3 eV	P antisite (+2/2+) level at cb + 1.3 eV	ODMR	[2]
E_4	cb − 0.14	Irradiation-induced electron traps	DLTS	[3–5]
E_5	cb − 0.16			
E_6	cb − 0.23			
E_7	cb − 0.37			
E_8	cb − 0.38			
E_9	cb − 0.54			
E_{10}	cb − 0.60			
E_{11}	cb − 0.76			
H_2	vb + 0.22	Irradiation-induced hole traps	DLTS	[4]
H_3	vb + 0.32			
H_4	vb + 0.37			
H_5	vb + 0.53			
H_6	vb + 0.23			
S_P	(0/+) cb − 0.0074	P-site donor	PL	[6]
Se_P	(0/+) cb − 0.0074	P-site donor		
Zn_{In}	$E(-/0)$ vb + 0.047	In-site acceptor	PL	[7, p 229]
Cd_{In}	$E(-/0)$ vb + 0.056	In-site acceptor		
Hg_{In}	$E(-/0)$ vb + 0.095	In-site acceptor		
DX		Donor-defect complexes with strong lattice coupling	DLTS, PL	[8]
M		Bistable donor–defect complex; strong lattice coupling; negative U	DLTS, PL	[9]

Defect label	Electrical level (V)	Model	Technique	Ref.
Cr	$E(0/-)$ vb + 0.94	In-site substitutional; transition-metal ions	ESR	[10]
Fe	$E(0/-)$ vb + 0.70			
Ni	$E(+/-)$ vb + 0.55			[6, 10]
Cu	$E(0/-)$ vb + 0.31	See section 2 for charge-state conventions		

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7. Group IV valence crystals

We concentrate on diamond, silicon and germanium, these being hosts for which a wealth of signals and representative traditional labels exist.

7.1. Defects in diamond

Here we give two main tables, one listing spin resonance signals (section 7.1.1) and one listing those optical transitions for which there are specific data that can be used to suggest models (section 7.1.2); e.g. isotope data indicating specific species are involved, or uniaxial stress data indicating symmetry. In addition, we give several lists that cross reference the different signals and labels; namely, commonly used labels to optical transition energies (section 7.1.3), specific impurity species to optical features (section 7.1.4) and spin resonance signals to optical features (section 7.1.5).

7.1.1. Defects observed in diamond using ESR and ODMR. The signals are ordered here alphabetically (and then numerically) according to their label. We follow the notation of Loubser and van Wyk [1] except where noted. Cross references to optical signals are given later.

Label	Spin	Model	Cross references
A	$s = 1$	Composite line?	S1, S2
A2, 3	$s = 1$	Radiation-induced defect formed at $T < 50$ K, or at $T \sim 300$ K after 1 year annealing!	[2]

Label	Spin	Model	Cross references
A4	$s = 1$	⟨111⟩ oriented N^- ion-implantation defect	
B	$s = 1$		R2
C	$s = 1$		R2
E1	$g \sim 4.2$	Co_i	[3]
N1	$s = 1/2$	N_s–C–CN_s	[5]
N2	$s = 1/2$	N-related	[5]
N3	$s = 1/2$	N-related	[5]
N4	$s = 1/2$	$(N–N)^+$ in plastically deformed brown diamonds; site of N atoms not certain	[4]
NL1	$j = 3/2$ h^+ state observed under stress	B_s acceptor	[4]
OK1	EPR: $s = 1/2$	N-related defect	
P1	$s = 1/2$; ENDOR	N_s; C_{3v} symmetry by repulsion of N_s from one bonded C	[2, 4]
P2	$s = 1/2$; ENDOR, ODMR	$3N_s$ + v complex with C_{3v} symmetry	N2, N3 optical bands
R1	$s = 1$		[2]
R2	$s = 1$		B
R3	$s = 1$		
R3	$s = 1$	Radiation complex involving vacancy?; correlates with TH5 optical band; ⟨111⟩ axis	TH5 (see later under optical signals)
R5	$s = 1$		
R6	$s = 1$	⟨110⟩ oriented v chain	
R7	$s = 3/2$	⟨110⟩ oriented v chain	
R8, 9, 10, 11	$s = 1$ or $3/2$	⟨110⟩ oriented v chain	
R12	$s = 1$ or $3/2$	⟨111⟩ oriented defect	
R15, 17	$s = 1/2$		
S1	$s = 1/2$	Vacancy related	A
S2	$s = 1/2$	N-related	A
S3	$s = 1/2$		
S4	$s = 1/2$		
W1, 2, 3	$s = 1$	⟨110⟩ oriented defect	
W4, 5		⟨110⟩ oriented radiation defect	

Label	Spin	Model	Cross references
W6	$s = 1$		R4
W7	$s = 1/2$	$(N–C–N)^+$ or $(N–C–C–N)^+$	
W8		Ni-related?	
W9	$s = 1$	⟨110⟩ oriented defect	
W10	$s = 2$	⟨111⟩ oriented defect (neutral chromium?)	
W11–14	$s = 1$	New ⟨111⟩ radiation defect (apparently rare)	
W15	$s = 1$ under visible illumination, $h\nu \gtrsim 1.95$ eV	N_s–v defect; C_{3v} symmetry; resonance in ^3E state	1.945 eV
W16, 17		Near ⟨111⟩ oriented radiation defect (apparently rare)	
W19	Radiation damage complex		
W20	$s = 1/2$	Radiation damage complex	
W21	$s = 1/2$	Three N atom complex in [110] plane	
W24	$s = 1/2$	⟨111⟩ structure involving two N_s atoms	A
W25	$s = 1$ under UV illumination	⟨110⟩ structures involving four N atoms?; v(s)?	H4
W26	$s = 1$ under UV illumination	⟨110⟩ symmetry; two equivalent N atoms	H3
W27, 28	$s = 1$	N-related	
W30	$s = 1/2$	⟨111⟩ axial arrangement of five N_s atoms	
W31	$s = 1/2$	Sulphur-associated	

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7.1.2. Opticals centres in diamond. The signals are ordered alphabetically (and then numerically as necessary) according to their label. Cross references are given in later tables. We follow Davies [1] unless otherwise stated. Energies of zero phonon lines are indicated by ZPL.

Label	Signals	Model	Cross reference
A	Luminescence (broad band in visible; variable peak energy)	Donor–acceptor pair (nitrogen–B_s)	
A	Absorption at $h\nu < 1332\,cm^{-1}$ and $h\nu > 3.765$ eV; photoconductivity at $h\nu > 3.76$ eV	N_s–N_s pair	
B	Absorption at $h\nu < 1332\,cm^{-1}$	N-related native defect	
b	Absorption at $h\nu < 1332\,cm^{-1}$ and $h\nu = 1340\,cm^{-1}$; continuum of absorption at $h\nu > 1.7$ eV	N_s	[2], C
C	Absorption at $h\nu < 1332\,cm^{-1}$ and $h\nu = 1340\,cm^{-1}$; continuum of absorption at $h\nu > 1.7$ eV	N_s	[2], b
D	Absorption at $h\nu < 1332\,cm^{-1}$	N-associated defect	[3]
D_0	Luminescence	Exciton bound to B_s	
GR1	Absorption; luminescence; ZPL = 1.673 eV	Neutral vacancy v^0; T_d symmetry; E to T transition	
GR2	Absorption; ZPL = 2.880 eV	v^0; transitions to higher excited T states of v^0	
GR3	Absorption; ZPL = 2.887 eV		
GR6a	Absorption; ZPL = 2.958 eV		
GR6b	Absorption; ZPL = 2.960 eV		
GR7a	Absorption; ZPL = 2.976 eV		
GR7b	Absorption; ZPL = 2.981 eV	Radiation complex involving N giving localised mode of variation	
H1a	Absorption at 0.181 eV	Radiation complex involving N giving localised mode of variation	
H1b	Absorption at 617 meV	Radiation complex involving N_s–N_i	[4], A
H1c	Absorption at 640.8 meV	Radiation complex involving the B centre	[4], B
H2	Absorption; ZPL = 1.25 eV	Radiation complex + nitrogen	
H3	Absorption; luminescence; ZPL = 2.463 eV	N_s + vacancy N_s; C_{2v} symmetry	W26 ESR signal
H4	Absorption; luminescence; ZPL = 2.498 eV	B nitrogen aggregate + vacancy	W25 ESR signal

Label	Signals	Model	Cross reference
H13	Absorption at 3.361 eV	Transition to excited state of H3 centre	H3
N2	Absorption at 2.596 eV	Vibronically induced band at N3 centre	N3
N3	Absorption; luminescence	$N_s + N_s + N_s$ + vacancy; C_{3v} symmetry	P2 ESR signal
N4	Absorption at 3.603 eV	Transition to excited state of N3 centre?	N3
N5, N6	Absorption; photoconductivity; ZPL = 3.765 eV	N_s–N_s	A
N9	Absorption; luminescence; photoconductivity; ZPL = 5.251–5.261 eV	N-related complex?	
ND1	Absorption; photoconductivity; ZPL = 3.150 eV	Negative vacancy v^-; T_d symmetry	R10
R10	Absorption; photoconductivity; ZPL = 3.150 eV	Negative vacancy v^-; T_d symmetry	ND1
R11	Absorption at 3.99 eV		[17]
S1	Luminescence and luminescence excitation	In naturally occurring diamond	[5]
TH5	Absorption, $h\nu \gtrsim 2.543$ eV	Divacancy?	R4 ESR signal
0.165 eV	Absorption	$k = 0$ optical vibration induced by Ni	[14]
0.305 eV 0.363 eV	Absorption; photoconductivity; photothermal ionisation	Substitutional acceptor; internal transitions and ionising transitions of h^+ on B_s	A, D_0
1.401 eV	Absorption; luminescence	Ni-associated centre	[6]
1.575 eV	Luminescence		[16]
1.673 eV	Absorption; luminescence	E (ground) to T (excited) state transition at v^0; T_d symmetry	GR1, 21
1.681 eV	Absorption; luminescence	Two interstitial Si atoms?	[15]
1.883 eV	Absorption	Ni-related defect	[14]
1.945 eV	Absorption; luminescence; photoexcited EPR	^1A (ground) to ^1E (excited) state transition at v–N_s; C_{3v} symmetry; EPR in ^3E state	[7], W15 ESR signal
2.086 eV	Absorption	E to E transition at C_{3v} defect; radiation damage complex + N?	2.918 eV

Label	Signals	Model	Cross reference
2.133 eV	Luminescence	Monoclinic II; naturally occurring defect	2.156 eV 2.166 eV
2.145 eV	Luminescence	Monoclinic I centre; naturally occurring defect	
2.156 eV	Luminescence	Monoclinic II centre; naturally occurring defect; similar to:	2.133 eV 2.166 eV
2.156 eV	Absorption; luminescence	E (ground) to A (excited) state transition at a C_{3v} defect; radiation damage complex + N	
2.166 eV	Luminescence	Monoclinic II centre; naturally occurring defect; similar to:	2.133 eV 2.156 eV
2.424 eV	Luminescence	Monoclinic II centre; naturally occurring	[8]
2.462 eV	Absorption; luminescence	Rhombic I defect; radiation complex	3H
2.463 eV	Absorption; luminescence	N_s–v–N_s; C_{2v} symmetry	H3 W26?
2.499 eV	Absorption; luminescence	Vacancy + 'B' nitrogen aggregate; C_{1h} symmetry	H4 W25
2.51 eV	Absorption	Ni-related	[14]
2.526 eV	Luminescence	N3-like band in plastically deformed regions	[9]
2.56 eV	Absorption	Ni-related	[14]
2.649 eV	Luminescence	Rhombic I defect; naturally occurring; similar to:	2.699 eV 2.748 eV 2.721 eV
2.699 eV	Luminescence	Rhombic I defect; naturally occurring; similar to:	2.649 eV 2.721 eV 2.748 eV
2.721 eV	Luminescence; luminescence excitation	Monoclinic I defect; naturally occurring; similar to:	2.649 eV 2.699 eV 2.748 eV
2.748 eV	Luminescence	Monoclinic I defect; naturally occurring; similar to:	2.649 eV 2.699 eV 2.721 eV

Label	Signals	Model	Cross reference
2.985 eV	Absorption; luminescence; ODMR	A (ground) to E (excited) state transition at [$N_s + N_s + N_s$ + v]; C_{3v} symmetry	N3; P2 ESR signal
3.1 eV	Absorption	Ni-related	[14]
3H	Absorption; luminescence	Rhombic I defect; radiation damage complex	2.462 eV
3.118 eV	Absorption	N-related radiation damage complex	[12]
3.20 eV	Luminescence	A to E transition at trigonal naturally occurring defect	3.224 eV
3.224 eV	Luminescence	Monoclinic I; naturally occurring defect	3.20 eV
4.059 eV	Absorption	Transition at N_s	[10], b, 4.567 eV
4.567 eV	Absorption	Transition at N_s?	[10], b, 4.059 eV
5RL	Absorption; luminescence; ZPL = 4.582 eV; local modes in vibronic sideband with $\hbar\omega \sim 237$ meV (in luminescence)	Radiation complex with rhombic I point group; carbon atom vibrating	[13]
1405 cm^{-1} 3107 cm^{-1}	Absorption	Local mode vibrations at defects involving H	
1450 cm^{-1}	Absorption	Local mode vibration produced by radiation damage, involving N	[11]

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7.1.3. Optical transitions in diamond. This list cross references commonly used labels to the energies of the optical features.

Name	Energy (eV)	Name	Energy (eV)
A, A′	5.246, 5.253	N3	2.985
B, B′	5.268, 5.275	N4	3.603
C, C′	5.322, 5.329	N5, 6	3.765, 3.933
D_0	5.356	N7, 8	4.050, 4.19
		N9	5.251
E_0	5.135	R9	3.04
GR1	1.673	R10	3.150
GR2, 3, 4	2.881, 2.888, 2.902	R11	3.988
GR5, 6, 7	2.940, 2.958, 2.976	S0	5.258
GR8	2.997	S1	2.463
H1a, b, c	0.181, 0.617, 0.641	S2	2.371
H2	1.25	TH5	2.543
H3	2.463	TR12	2.638
H4	2.499	TR14	2.777
H13	3.311		
M1	2.400	TR15	2.788
M2	2.445	TR16	2.817
ND1	3.150	TR17	2.831
N1	1.50	3H	2.462
N2	2.596	5RL	4.582

7.1.4. Optical transitions in diamond. This list cross references from impurity species to energies of optical features.

Element (defect)	Transition energy
B (boron)	Characteristic bands in one-phonon region, $0 < h\nu < 0.165$ eV plus transitions to shallow excited states at 0.305 eV, etc.
H (hydrogen)	0.174 eV
N (nitrogen)	Characteristic bands in one-phonon region, $0 < h\nu < 0.165$ eV
Single nitrogen atom	4.137 eV
Paired nitrogen atoms	3.765 eV
v^0 neutral vacancy	1.673, 2.881 eV, etc.
v^- negative vacancy	3.150 eV
N–v	1.945 eV
N_2–v	2.463 eV
N_3–v	2.985 eV

7.1.5. Optical transitions and spin resonance signals. This list cross references spin resonance and optical features associated with the same defect.

ESR label	Optical label
P2	N2, N3, 2.985 eV
W15	1.945 eV
W25(?)	H4
W26	H3 (also H13)
R4(?)	TH5

7.2. Defects in silicon

Here it is convenient to list signals in several ways. Our first table (section 7.2.1) is analogous to those for III–V and II–VI semiconductors, listing defects seen in spin resonance and transient spectroscopy. These relate to defect ground states and to transitions that change the defect charge state. The second table (section 7.2.2) lists the sharp lines (which are either zero-phonon lines or similar in appearance). There are then several tables that allow cross reference, listing photoluminescence bands by their labels (section 7.2.3), and vibrational lines from infrared absorption (section 7.2.4), comprising an alphabetical list of lines with labels and a further list in order of energy, and finally defect and signal labels (section 7.2.5). Nn means nearest-neighbour.

7.2.1. Defects seen in ESR and DLTS

Defect label	Electrical level (V)	Model	Technique	Ref.
v	$E(0/2+)$ vb + 0.09	Monovacancy; JT distorted	ESR, DLTS	[1, 2]
	$E(0/+)$ vb + 0.05 $E(+/2+)$ vb + 0.13	Negative U; $v^+ = D_{2d}$ bond-pairing distortion (Si–G1)		
	$E(-/0)$ mid-gap $E(2-/-)$ upper gap	Positive U; $v^- = D_{2d} + C_{2v}$ distortion (Si–G2)		
v_2	$E(2-/-)$ cb − 0.25 $E(-/0)$ cb − 0.41 $E(0/+)$ vb + 0.25	Nn divacancy Small reconstruction v_2^+ = Si–G6, v_2^- = Si–G7	ESR DLTS	[3–6]
v_3 v_4 v_5		Multivacancies	ESR	[7]
P	E(0/+) cb − 0.0455	Substitutional donor	IR, ESR, ENDOR	[8, p 156]
As	$E(0/+)$ cb − 0.0537			
Sb	$E(0/+)$ cb − 0.0427			
Bi	$E(0/+)$ cb − 0.071			
N	$E(0/+)$ upper gap	SL-5, C_{3v} distortion; unpaired electron in Si dangling-bond-like orbital; electrical level uncertain	ESR	[9]

Defect label	Electrical level (V)	Model	Technique	Ref.
S	$E(0/+)$ cb − 0.3182 $E(+/2+)$ cb − 0.6132	Substitutional double donor	IR, ESR, ENDOR	[10, 11]
Se	$E(0/+)$ cb − 0.3015 $E(+/2+)$ cb − 0.5932			[8, 10, 11]
Te	$E(0/+)$ cb − 0.1987 $E(+/2+)$ cb − 0.4112			
Li	$E(0/+)$ cb − 0.031	T_d interstitial donor	IR	[8, p 163; 12]
Mg	$E(0/+)$ cb − 0.108 $E(+/2+)$ cb − 0.256	T_d interstitial donor		[8, p 163]
B	$E(0/-)$ vb + 0.045	Substitutional acceptor	IR, ESR	[8, p 166]
Al	$E(0/-)$ vb + 0.057			
Ga	$E(0/-)$ vb + 0.065			
In	$E(0/-)$ vb + 0.16			
Tl	$E(0/-)$ vb + 0.25			
B_i	$E(+/-)$ cb − 0.29	Bonded interstitial of unsettled configuration Si–G28	DLTS, LESR	[1, 13, 14]
	$E(+/0)$ cb − 0.13 $E(0/-)$ cb − 0.45	Negative U		
Al_i	$E(0/+) \sim$ cb − 0.1 $E(+/2+)$ vb + 0.17	T_d interstitial; Al^{++} is Si–G18	ESR, DLTS	[15, 16]
Si_i	?	Si–G25 signal, debated	ESR	[17, 18]
C_i	$E(-/0)$ cb − 0.09 $(0/+)$ vb + 0.27	⟨100⟩ split interstitial with trivalent C, Si sites; Si–G12		[19, 20]
C_i–C_s		Si–G11; two carbon analogue of L_i		[21]
C_iO_i	vb + 0.36	C_i radiation damage complex trapped at O_i	DLTS	[20]
C_iC_s	$(-/0)$ cb − 0.17 $(-/0)$ cb − 0.10 $(0/+)$ vb + 0.09 $(0/+)$ vb + 0.05	Metastable states of C_i trapped at substitutional C		[20]
N–N	? vb + 0.66	Nitrogen pair, structure uncertain		
O_i	None	Puckered, bond-centred interstitial	IR	[8, p 180]
S_2	$E(0/+)$ cb − 0.1875 $E(+/2+)$ cb − 0.371	Nn donor pair	IR, ESR	[10, 11]
Se_2	$E(0/+)$ cb − 0.2064 $E(+/2+)$ cb − 0.39			
Te_2	$E(0/+)$ cb − 0.158			

Defect label	Electrical level (V)	Model	Technique	Ref.
$S_c(X_1)$	$E(0/+)$ cb + 0.1095 $E(+/2+)$ cb − 0.248	Chalcogen pair-defect complexes		[10, 11]
$S_c(X_2)$	$E(0/+)$ cb − 0.092			
$S_c(X_3)$	$E(0/+)$ cb − 0.082			
$S_c(X_4)$	$E(0/+)$ cb − 0.0806			
$S_c(X_5)$	$E(0/+)$ cb − 0.0565			
$Se_c(X_1)$	$E(0/+)$ cb − 0.1159 $E(+/2+)$ cb − 0.214			
$Se_c(X_2)$	$E(0/+)$ cb − 0.0941			
$Se_c(X_3)$	$E(0/+)$ cb − 0.053			
$Te_c(X_1)$	$E(0/+)$ cb − 0.1268	Chalcogen pair-defect complexes		
$Te_c(X_2)$	$E(0/+)$ cb − 0.1098			
$Te_c(X_3)$	$E(0/+)$ cb − 0.0933			
$Te_c(X_5)$	$E(0/+)$ cb − 0.0653			
O_n	$E(0/+)$ cb − 0.06 $E(+/2+)$ cb − 0.15	Oxygen-related thermal donor (TD) family; C_{2v} clusters of five or more oxygens; possibly TD^+ = NL8	DLTS, ESR, IR ENDOR	[11, 22] [23]
v–P	$E(0/-)$ cb − 0.45	Nn vacancy–phosphorus pair (E centre), Si–G8; P dangling bond doubly occupied; two Si dangling bonds re-bond; unpaired electron on third Si	ESR	[9, 17]
v–As	$E(0/-)$ cb − 0.42	Nn v–As pair (Si–G23)	ESR	[9, 17]
v–Sb	$E(0/-)$ cb − 0.39	Nn v–Sb pair (Si–G24)	ESR	[9, 17]
v–Bi	$E(0/-)$	Nn v–Bi pair		[9, 17]
v–O	$E(0/-)$ cb − 0.18 $E(+/0)$ lower gap?	Vacancy–O interstitial, C_{2v} (A centre); equivalent to severely off-centre O_{Si}; A^- is Si–G15; excited A^0 is Si–B1 with $s = 1$	ESR, DLTS	[8, p 185; 24, 25]
v–Ge	$E(0/+)$ $E(+/2+)$	Nn v–Ge pair		
v–Sn	$E(0/+)$ vb + 0.07 $E(+/2+)$ vb + 0.32	Nn v–Sn pair Weak JT, positive U; Si–G29		[1, 26]
v–Al	$E(-/0)$ vb + 0.48	Nn v–Al pair; Si–G9	ESR	[4, 27]
v–B		Two Nn v–B; Si–G10	ESR	[28]

Defect label	Electrical level (V)	Model	Technique	Ref.
Ti	$E(-/0)$ cb − 0.08 $E(0/+)$ cb − 0.28 $E(+/2+)$ vb + 0.25	Interstitial	DLTS	[29–32]
V	$E(-/0)$ cb − 0.16 $E(0/+)$ cb − 0.45 $E(+/2+)$ vb + 0.30	Interstitial vanadium	DLTS, ESR	
Cr	$E(0/+)$ cb − 0.22	Interstitial Cr^+, Cr^0 Substitutional Cr^0	DLT, ESR ESR	
Mn	$E(-/0)$ cb − 0.11	Interstitial Mn^{2+}, Mn^+, Mn^0, Mn^-		
	$E(0/+)$ cb − 0.42 $E(+/2+)$ vb − 0.25		DLTS, ESR	
	$E(0/+)$ vb + 0.38 $E(-/2-)$ upper gap?	Substitutional Mn^+, Mn^{2-}	ESR, DSTS	[33]
Fe	$E(0/+)$ vb + 0.38	Interstitial		[29–32, 34–37]
Co	$E(-/0)$ cb − 0.535 $E(0/+)$ vb + 0.38	Interstitial	DLTS	
Ni	$E(0/+)$ cb − 0.4 $E(-/0)$ vb − 0.22	Interstitial	ESR	
Au	$E(-/0)$ cb − 0.55 $E(0/+)$ vb + 0.34	Quasi-substitutional	DLTS	
Ag	$E(-/0)$ cb − 0.54 $E(0/+)$ vb + 0.29		DLTS	
Cu	$E(0/+)$ vb + 0.24		DLTS	
Pt	$E(-/0)$ cb − 0.23 $E(0/+)$ vb − 0.32	Substitutional Pt^0 is d^{10} Pt^- similar to (vacancy)$^-$	DLTS, ESR	[2]
Pd	$E(-/0)$ cb − 0.22 $E(0/+)$ vb + 0.33	Pd_I		[23]
	$E(-/0)$ vb + 0.32	Pd_{II}		[31]
X–B	$E(0/+) \sim$ vb + 0.1	Hole traps of transition-metal–boron complexes; X = Mn, Fe, Co, Ni, Cu, Zn; also Al, Ga, In complexes	ESR, DLTS	[32]
Fe–Al	$E(0/+)$ vb + 0.2	Fe_I–Al_{Si} complex; metastable levels; strong electron–lattice coupling		[38]
X–Au	~vb + 0.4	Hole traps of transition-metal–gold complexes; X = Ti, V, Cr, Mn, Fe, Co		[32]
C_iP_s	cb − 0.21 0.23 0.29 0.30	C_iP_s radiation damage complex in four metastable configurations	DLTS	[20]

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7.2.2. Sharp (zero-phonon-like) optical transitions in Si. In this list of sharp lines, luminescence lines are denoted L, absorption lines are denoted A and photoluminescence excitation lines are denoted PLE. Lines are in *decreasing* order of energy; the labels can be obtained from the subsequent cross reference tables. The list is based on the review by Davies [1].

Energy (meV)	Mode	Phonons (meV)	Model
1152.5	L		Zero-phonon emission from modified 1094.5 meV F centre; '1F'
1152	L		Zero-phonon emission from modified 1094.5 meV F centre; '2F'
1150.7	L	TO = 58	B bound exciton zero-phonon line
1150.1	L	TO = 58	Sb bound exciton zero-phonon line
1150.0	L	TO = 58	P bound exciton zero-phonon line Multibound exciton lines involving m excitons at: $m = 2$, 1146.5; $m = 3$, 1143.7; $m = 4$, 1141.7; $m = 5$, 1140.5; $m = 6$; 1139.3 meV
1149	L	TO = 58	Al bound exciton zero-phonon line Multiexciton zero-phonon lines for m excitons at: $m = 2$, 1146.3; $m = 3$, 1143.7; $m = 4$, 1141.5; $m = 5$, 1140.3 meV
1149.2	L		As bound exciton zero-phonon line
1149.0	L	TO = 58	Ga bound exciton zero-phonon line
1148.8	L		Zero-phonon emission at P donor; and associated line at 1147.9 meV; 'a1' and 'a2'
1146.9	L	TA = 19	Bi bound exciton zero-phonon line
1143.9	L	TO = 58	'S1' bound exciton line of sulphur
1143	L	TA = 19	'TD' produced in CZ silicon by heating at 450 °C (*not* thermal donors)
1142.2 etc.	L		H^+ implantation and anneal 450–600 °C
1141.0	L	TO = 58	In bound exciton line
1132.6	L		Emission from exciton bound to Li donor with Ta phonon creation
1131	L		Radiation damage in Si:Li 'Y'
1129.9	L		Emission from multibound excitons at Li donor involving two excitons; similar multiexciton emission involving m phonons at: $m = 3$, 1127.8; $m = 4$, 1125.9; $m = 5$, 1124.5; $m = 6$, 1123.2 meV
1129.8	L		Zn–implantation centre [2]
1126	L		Radiation damage in Si"Li"Z"
1122	A, L		Trigonal isoelectronic centre involving N + Al?; shallow h^+ with pseudo-acceptor binding energy 36.7 meV; 'ABC'
1117.6	L	66	'O1', one of a series, O2 = 1115.6, O3 = 1113.7, O4 = 1111.8 meV; thermally induced in CZ Si; asymmetric lineshape suggesting either a bound-to-free transition or strain broadening
1117.5	L, PLE	9.2	Monoclinic II, In-related; associated lines at 1115.9, 1108.5 meV; 'PQR' of In
1117	L		Radiation damage of Si:Li; 'X'
1117	L		Isoelectronic centre involving Be + C

Energy (meV)	Mode	Phonons (meV)	Model
1116.9	L		Strongest of three lines observed at 1116.1, 1116.9 and 1119.3 meV after B ion implantation; dependence on B isotope
1115.0	L		'SZ' bound exciton, perhaps at a sulphur defect
1108.3	L		First in the series of 'S' lines of which the other main lines are at: 1104.6, 1100.5, 1092.7, 1090.5, 1088.1, 1085.5, 1070.4, 1067.2, 1060.8, 1034.2, 1023.4, 1014.4 meV; formed in CZ Si by 100 h at 500 °C
1108.1	L		Produced by neutron irradiation of float-zone silicon and annealing at 250 °C
1107.2	L		'D1' observed after laser annealing
1100.6	L		Radiation damage centre produced by He^+, H_2^+, H^+ bombardment
1095	L		TO phonon sideband emission of exciton bound to modified 1094.5 meV F centre Multibound exciton emission from m excitons at: $m = 2$, 1092; $m = 3$, 1090; $m = 4$, 1088.5 meV; '3F'
1094.5	L		TO phonon sideband emission of exciton formed in CZ Si with $[C] > 5 \times 10^{16}\,cm^{-3}$ after heating; multi-bound exciton emission from m excitons at: $m = 2$, 1092.5; $m = 3$, 1090; $m = 4$, 1088.5; $m = 5$, 1087 meV; 'F'
1094.5	L		TO phonon sideband emission of exciton bound to modified 1094.5 meV F centre
1093.2	L		Emission from exciton bound to Li donor with TO phonon creation
1092.8	L	TO	Sideband of excitons bound to 'N–O' donors produced by N? + O? [3]
1092.7	L		Emission from exciton bound to B acceptor with TO phonon emission; multiexciton emission involving m excitons at: $m = 2$, 1090.4; $m = 3$, 1088.1; $m = 4$, 1086.5 meV
1091.9	L		Sb bound exciton and TO phonon emission
1091.8	L		P bound exciton and TO emission Similar multiexciton lines involving m excitons at: $m = 2$, 1088.2; $m = 3$, 1085.6; $m = 4$, 1083.7 meV
1091	L		As bound exciton and TO emission
1090.0	L		Multibound exciton emission involving two excitons on Li donor and TO phonon creation; similar multiexciton emission involving m excitons at: $m = 3$, 1088.5; $m = 4$, 1086.8; $m = 5$, 1085; $m = 6$, 1083.8; $m = 7$, 1082.5; $m = 8$, 1081.1 meV
1086.9	L		Tl-related lines, low T version ($T < 20$ K) Associated lines at 1081.5, 1080.4 meV

Energy (meV)	Mode	Phonons (meV)	Model
1082	A, L		Radiation damage of Si:(Cl + Li) and anneal at 300 °C; very similar to 1045 meV; 'S'
1081.1			Observed in B-implanted Si after 400 °C anneal
1080	L	30.2, local mode	Monoclinic I centre produced by B implant or electron irradiation of Si:B; involves two B atoms; local modes 11B = 104.6, 10B = 109.4 meV; '12'
1076	L		Si:Be isoelectronic centre; trigonal?
1067.2	L		One of the S series—see 1108.3 meV line
1067			Fe(?) related band: one-phonon induced transition of 'FeB'
1062.5	L		Produced by neutron irradiation and 300 °C anneal of CZ Si
1060	L		Radiation damage at 100 K involving C and O
1052	L		'D1' asymmetric line produced after heating CZ silicon at 500 °C; *not* thermal donors
1050.2	L		Ga-related radiation damage centre Singlet line of singlet–triplet pair, triplet at 1047.2 meV; 'Ga-2'
1050.1			Tl-related lines observed at $T > 15$ K Other lines at 1048, 1042.7 meV; 'T1 PWR'
1049	L		Radiation damage of Si:Ga and anneal 250 °C
1045	A, L	32.2, 47.9, 55.1	Radiation damage of Si:Li; trigonal centre of four Li atoms (at vacancy?) Singlet line of singlet–triplet pair, triplet at 1044 meV; excited state at 1048 meV; 'Q'
1039.8	L		Ion implantation, neutron damage and anneal at 500 to 800 K; tetragonal A to A or tetrahedral A to T transition; '13' or 'X'
1037	L		Produced by ion bombardment
1034.2	L		One of the S series—see 1108.3 meV S line
1025	L		Produced in e-irradiated FZ Si:Li and 450 °C anneal
1023.4	L		One of the S series—see 1108.3 meV S line
1018.3	L		Ion implantation (or similar) damage line; trigonal centre, A to A transition; 'I1' or 'W'
1014.8	L		Line like 1018.3 meV W but produced by Ne implantation
1014.7	L	7	Cu-related trigonal centre
1014.4	L		One of the S series—see 1108.3 meV S line
1012	L		Line like 1018.3 meV W but produced by He implantation
1010.3	L	15	See 707 meV
1009.7	L		Line like 1018.3 meV W but produced by Ar implantation; A to A transition at trigonal centre

Energy (meV)	Mode	Phonons (meV)	Model
1004.8	L		Line like 1018.3 meV but produced by Kr implantation
1003.7	L		Rhombic I centre produced by neutron irradiation and 400 °C anneal in CZ Si
1000	L		Produced by Xe implantation
997	L		Dislocation-related centre; 'D4'
990 ±10	L		Ion implantation damage and hydrogenation
996.8	L		Produced by neutron irradiation and anneal at 150 °C
988.8	L		Produced by neutron irradiation and 375 °C anneal ('K')
986.2	L		S–related; triplet state with singlet at 977.1 meV [4]
977.8	A, L		Observed in sulphur-doped Si
969.5	A, L, P DLTS, ODMR	15	Monoclinic I centre involving two C and one unique Si atom, 'B'
967.4	L		Produced by neutron irradiation and anneal at 150 °C
965.2	L		Produced by 450 °C heating of CZ Si; 'I'
957	L		Produced in CZ Si by 180 h at 450 °C or by irradiation damage below 200 °C? Same centre?
956.9	L		Perturbed form of 969 meV G
953.9	L		Perturbed form of 969 meV G
953	L		Perturbed form of 696 meV G ('E')
951.2	L		Perturbed form of 969 meV G
949.9	L		C-related radiation damage centre, monoclinic I symmetry
947	L		Produced by radiation damage and 450 °C anneal
944.8	L	10.3, *G*	Observed in (Mn + Zn)-doped Si
943.7	L	6.4	Observed after Cu diffusion, trigonal centre
939	L		Dislocation-related centre; 'D3'
935.2	L		Produced by radiation damage at 20 °C in C-doped float-zone silicon
935.1	L	129.4, 66.3	Rhombic I centre involving C produced by radiation damage and anneal at 450 °CC; 'T'
929.1	L		C-related radiation damage centre
929	L	59.4	⟨100⟩ symmetry axis? Singlet of singlet–triplet system; 'Ga3'
926	L		Radiation damage and anneal at 250 °C of Si:Ga
925.5	L		Radiation damage centre involving C

Energy (meV)	Mode	Phonons (meV)	Model
922.3	L		Produced by high T anneal involving Al? + C?
919.8	L		Radiation damage centre involving C
903	L		Produced by 300–400 h at 450 °C in CZ Si
897.9	L		Produced by radiation damage of CZ Si and anneal at 350 °C
878	L		Produced by radiation damage and anneal at 100 °C of Si:Li
875	L	55.8	Radiation damage of Si–Ga involving C in a rhombic I centre; 'Ga1'
874	L		Dislocation-related tetragonal centre; 'D2'
868.7	L		Induced by As implantation during growth of MBE silicon at 500° C [5]
856	A, L		Rhombic I C interstitialcy
844	L	14, G	Observed after Cr diffusion into Si:B
836	L		Rhombic I radiation damage centre produced in Si:Al; 'Al 1'
829.8	A	15	Au-related centre?
811.1, 810.5	L	Resonances at 7.2, 9.2 and 16.5	Rhombic I centre produced by Pt(?) diffusion
808.8	L		Observed in MBE silicon
807	L		Dislocation-related tetragonal centre; 'D1'
805.4	L, PLE	15	Produced by Pt(?) diffusion; T_d or tetragonal symmetry
797.6	L		Metastable form of 775.1 meV Al centre?
793.4, 793.0, 792.8, 791.9	L	3, 7	Au(?) associated
789.4	A, L	TA = 19, 65.5, 72.5, 138.1, 145	Monoclinic I radiation damage centre involving C and O; shallow donor e^- state; 'C'
785	L		Produced by radiation damage and 300 °C anneal of Si:Li
775.1	L		Room-temperature irradiation product with tetragonal symmetry? in Si:Al
772.4			'N5'—see 745.6 meV N1
768.6	L		C-related radiation damage centre
767.4	L, A		'N4'—see 745.6 meV N1

Energy (meV)	Mode	Phonons (meV)	Model
767.3	A, L	TA = 18, LA = 43, 65.6, 72	Monoclinic IC-related centre produced by radiation damage and annealing at 450 °C in CZ Si; shallow effective-mass-like e^- with binding energy 34 meV; 'P'
766.7	L		Produced by neutron irradiation in CZ Si
761.5	L		'N3' C, N, O complex
760.6	L		Radiation damage centre involving C; 'M'
758	L		'N2' C, N, O complex
745.6	L	122.9 71.3	Monoclinic I centre involving N and C atoms; deep h^+, shallow e^- states; 'N1' line; related lines N2 . . . N5
737.6, 735.1, 734.7	L	7.5, 10	Observed after Fe(?) diffusion
707	A	15	Au-related centre?
698	A	15	Radiation damage involving C? and O? [7]
677	L		Observed after Cr diffusion into Si:Ca
615	L	18.5	Trigonal centre in MBE silicon
567.9	L		See 564.7 meV
566.1			See 564.7 meV
565.7			See 564.7 meV
564.7	L	13, ~60	Mn related? tetrahedral? centre
488	A, L		Monoclinic I centre, radiation damage centre, involving C and O

[1] Davies G 1989 *Phys. Rep.* **176** 83
[2] Henry M O, Campion J D, McGuigan, Thewalt M W L and Lightowlers E C 1989 *E-MRS Conference*
[3] Steele A G, Lluchyshyn L C and Thewalt M W L 1990 *Appl. Phys. Lett.* **56** 148
[4] Singh M, Lightowlers E C, Davies G, Jeynes C and Reeson K J 1989 *Mater. Sci. & Eng.* B **4** 303
[5] Rowell N L 1989 *Thin Films* **182** at press
[6] de Mello, Davies G, Lightowlers E C, Higgs V, Gibbings C J and Tupplu C G 1989 *Thin Films* **182** at press
[7] Svensson J H and Monemar B 1989 *Phys. Rev.* B **40** 1410

7.2.3. Photoluminescence bands in silicon: list by labels

Label	Energy (meV)	Model
ABC	1122	C_{3v} isoelectronic centre involving N–Al pair (?)
Al 1	836	Tetragonal centre(?) with singlet–triplet excited states

Label	Energy (meV)	Model
C	789.4	C_{1h} C–C complex produced by radiation damage; same centre at C(3) vibrational centre; diamagnetic state of Si–G15
D1	807	Dislocation-associated luminescence at tetragonal centre
D2	874	Dislocation-associated luminescence at tetragonal centre
D3	939	Dislocation-associated luminescence
D4	997	Dislocation-associated luminescence
G	969	≡C—Si—C≡ complex; C_{1h} symmetry; diamagnetic state of Si–G11
Ga1	875	C_{2v} radiation damage complex in Si:Ga involving carbon
Ga2	1047	Radiation-induced in Si:Ga
Ga3	929	Tetragonal centre (?) with singlet-triplet excited states
H	925.9	Radiation damage and anneal at 450 °C in CZ (Czochralski growth method) Si, involving carbon (?)
I_2	1080	C_{1h}, B implant or radiation damage of Si:B
I1(W)	1018	C_{3v} complex produced by radiation damage from heavy ions, neutrons, etc
I3(X)	1040	T_d or tetragonal complex produced by radiation damage from heavy ions, n^0, etc.
M	760.6	Radiation damage involving carbon
N1	746	C_{1h} N–C structure
O1	1118	Transition of electron at thermal donor to vb; centre produced by heating CZ Si at 450 °C
P	767.3	C_{1h} radiation damage produce in CZ Si, involving carbon
PQR	1108–1118	In-related lines
Q	1045	Four Li atom complex in C_{3c} symmetry, produced by radiation damage
S	1082	Radiation damage complex in Si:(Li + C), a carbon-modified version of Q
S_n ($n = 1$ to 19)	~1000–1100	C + O associated lines produced by heating CZ Si
Tl PQR	1043–1050	Tl-related lines observed at $T > 15$ K

7.2.4. Vibrational lines in silicon, observed by infrared absorption. Lines are listed in limit of low temperature, for the most abundant isotopes.

Label	Energy (cm^{-1})	Model
A	836	V–O, i.e. off-site substitutional O atom

Label	Energy (meV)	Model
C(s)	607	Substitutional carbon; line used as a calibration for carbon concentration
C(1)	921,930	C_i, C_{3v}(?) symmetry
C(3)	865,1115	C–O complex; same centre as C photoluminescence band; diamagnetic state of Si-G15 centre
C(4)	1020	C–O complex of C(3) plus self-interstitial

Energy (cm^{-1})	Model
518	O_i
564,657	B_s–Li_i substitutional B and interstitial Li in C_{3v} complex
589,640	C–O pair in as-grown Si
600,628	B_s–P_s substitutional pair
604,637	B_s–As_s substitutional pair
607	C_s; used as calibration line for carbon concentration
612,643	B_s–Sb_s substitutional pair
623	B_s
766,963	N–N pair in uncertain configuration
836	V–O (A centre) in neutral charge
865,1115	C–O radiation-induced complex; same centre as 789 meV photoluminescence centre C and diamagnetic state of Si-G15
884	V–O in negative charge state
884	VO_2
930,921	C_i, stable at $T = 300$ K in C_{3v}(?) symmetry
969	VO_3
1104	C–O pair
1136 (etc.)	O_i multiple lines forming the 9 μm band; used as calibration for O concentration

7.2.5. Defect and signal labels: cross reference. Our list contains two types of labels, namely those of defects and signals. The present list is alphabetical by signal. A blank means no defect model is clearly identified for the signal.

B1	$v^{-0}(A^0)$	NL5	
NL1		NL6	
NL2		NL7	
NL3		NL8	O_n thermal donor?
NL4		G1	v

G2	v	G16	
G3		G17	
G4		G18	Al_i
G5		G19	
G6	v^2	G20	
G7	v^2	G21	
G8	v^2–P(E)	G22	
G9	v–Al	G23	v–As
G10	v–B	G24	v–Sb
G11		G25	Si_i?
G12	C_i	G26	
G13		G27	
G14		G28	B_i
G15	v–O (A^0)	G29	v–Sn

7.3. Defects in germanium

Note that no intrinsic defects are listed, since the situation is far less clear than for silicon. It is reasonably certain that the neutral (v^0) and negative (v^-) vacancies occur.

Defect	Electrical level (V)	Model	Technique	Ref.
P	$E(0/+)$ vb + 0.01276	Substitutional donor	IR	[1]
As	$E(0/+)$ vb + 0.01404			
Sb	$E(0/+)$ cb − 0.01019			
Bi	$E(0/+)$ cb − 0.01268			
Li	$E(0/+)$ cb − 0.00989	Interstitial donor		
B	$E(-/0)$ vb + 0.01047	Substitutional acceptor		
Al	$E(-/0)$ vb + 0.1080			
Ga	$E(-/0)$ vb + 0.1097			
In	$E(-/0)$ vb + 0.01161			
Tl	$E(-/0)$ vb + 0.0131			
Be	$E(-/0)$ vb + 0.02445 $E(2-/-)$	Acceptor		
Zn	$E(-/0)$ vb + 0.03263 $E(2-/-)$ vb 0.0858			
Cd	$E(-/0)$ vb + 0.0541 $E(2-/-)$			
Hg	$E(-/0)$ vb + 0.0915 $E(2-/-)$			
Cu	$E(-/0)$ vb + 0.0428			

[1] Ramdas A K and Rodriguez S 1981 *Rep. Prog. Phys.* **44** 1297

8. Other systems

Here we collect together a number of other systems for which there are adopted defect labels. Clearly, such lists could be extended substantially by including more and more limited usages. The examples we include are representative of labelling conventions quite widely applied.

8.1. Amorphous semiconductors

The convention in these tables is that a *defect* refers to any miscoordinated atom and the labelling convention is of the form X_n^q where X labels a species (C = group VI chalcogen, P = group V pnictide and T = group IV species), q refers to the charge (see also section 2) and n gives the coordination.

We list three systems here, namely amorphous silicon (hydrogenated, i.e. a-Si:H) (section 8.1.1), amorphous As_2Se_3 (section 8.1.2) and amorphous silicon nitride (section 8.1.3). Note that amorphous silica was covered in section 5, along with the related crystalline oxide.

8.1.1. Hydrogenated amorphous silicon, a-Si:H. These cases can be compared with the corresponding c-Si cases in section 7.2.

Defect label	Electrical level (V)	Model	Technique	Ref.
Si_3	$E(-/0)$ cb − 0.8 $E(0/+)$ cb − 1.2	Silicon dangling bond site (≡Si) $g = 2.0055$	DLTS, ESR	[1–3]
P_4	$E(0/+) \sim$ cb − 0.15	Substitutional donor	ESR	[4]
As_4	$E(0/+) \sim$ cb − 0.2	Substitutional donor	ESR	[4]
B_4	$E(-/0) \sim$ vb + 0.15	Substitutional acceptor		
e	cb	Band tail electron, $g = 2.004$	ESR	[2]
h	vb	Band tail hole, $g = 2.011$ ('A centre')	ESR, ODMR	[2, 5]
Defects of *Staebler–Wronski effect*	Mid-gap	Light-induced metastable defects (≡Si^0) and perhaps other centres		[6–8]
1.3 eV		Band tail–band tail luminescence	PL	[2]
0.9 eV		Band tail–dangling bond luminescence	PL	[2]

[1] Lang D V, Cohen J D and Harbison J P 1982 *Phys. Rev.* B **25** 5285
Winer K 1989 *Phys. Rev. Lett.* **63** 1437
[2] Street R A, Biegelsen D K and Knights J C 1980 *Phys. Rev.* B **24** 969
[3] Stutzman M and Biegelsen D K 1988 *Phys. Rev. Lett.* **60** 1682
[4] Stutzman M and Street R A 1987 *Phys. Rev.* B **35** 5666
[5] Morigaki K 1983 *J. Phys. Soc. Japan* **27** 375

[6] Staebler D L and Wronski C R 1977 *Appl. Phys. Lett.* **31** 292; Wronski C R 1988 *Physics and Applications of Amorphous Semiconductors* ed F Demichelis (Singapore: World Scientific) p 291
[7] Stutzman M, Jackson W B and Tsai C C 1985 *Phys. Rev.* B **32** 23
[8] Stutzman M 1988 *Festkörperprobleme* (*Advances in Solid State Phys.*) vol 28, ed P Grosse (Braunschweig: Vieweg) p 1

8.1.2. Amorphous As_2Se_3

Defect label	Electrical level (V)	Model	Technique	Ref.
Se_1^0		Se dangling bond	LESR	[1, 2]
As_2^0		As dangling bond	LESR	[1, 2]

[1] Bishop S G, Strom U and Taylor P C 1977 *Phys. Rev.* B **15** 278
[2] Robertson J 1983 *Adv. Phys.* **32** 361

8.1.3. Amorphous silicon nitride

Defect label	Electrical level (V)	Model	Technique	Ref.
Si_3^0		Silicon dangling bond	ESR	[1]
N_2^-		Negative N dangling bond		

[1] Robertson J and Power M J 1984 *Appl. Phys. Lett.* **44** 415
[2] Krick D T, Lenahan P M and Kanicki J 1988 *Phys. Rev.* B **38** 8226

8.2. Muonium in non-metals

Implanted positive muons (μ^+) in solids readily capture an electron to form a complex [μ^+e]; other species can occur too, but this 'muonium' complex is observed most readily and has been systematically studied. Recent data are reviewed by Cox [1]. One striking feature of these data is that there are two main distinct types of interstitial muonium:

Mu′	(previously 'normal' muonium), in which the electron is relatively well localised (almost certainly at a tetrahedral interstitial site) and of high symmetry, resembling the free-space complex)
Mu*	(previously 'anomalous' muonium), in which the muon is almost certainly at a bond-centre site; there is considerable anisotropy (with (111) symmetry in systems like Si and Ge) and a low electron density at the muon
Mu	is now reserved as a label for the free-space muonium complex
Mu″	(also in two forms Mu I and Mu II observed in CuCl) is a further generalisation in which the muon tunnels between several sites, at each site exhibiting some degree of hybridisation with a Cu^+ cation

[1] Cox S F J 1987 *J. Phys. C: Solid State Phys.* **20** 3187

8.3. Ice

In ice, as in the amorphous semiconductors of section 8.1, the defects in ice are those which break certain structural rules. There are, in fact, analogies between ice (H_2O) and silica (O_2Si), though the data for ice are much less complete or sophisticated [1]. The structural rules for ice are (i) that there are two hydrogens close to each oxygen and (ii) that, on the line joining any two oxygens, there is only a single hydrogen.

Violations of rule (i) lead to the *ionisation defects*, namely:

H_3O^+	Corresponding to C_3^+ in chalcogenide glasses
OH^-	Corresponding to C_1^- in chalcogenide glasses

Violations of rule (ii) lead to the *Bjerrum defects*:

D defects	Two hydrogens on an oxygen–oxygen join
L defects	No hydrogens on an oxygen–oxygen join

[1] Hobbs P V 1974 *Ice Physics* (Oxford: Oxford University Press)

8.4. Conducting polymers: polyacetylene and related conjugated chains

These systems, the simplest being hydrocarbon chains like the polyacetylenes $(CH)_N$, show a range of behaviour—which includes electron–phonon coupling, p-type and n-type doping, carrier trapping and the concepts more novel to physicists than chemists of isomerisation (as in the existence of both *trans* and *cis* forms of polyacetylene) and of bond alternation (equivalent to a Peierls distortion for *trans*-polyacetylene). Figures 1 and 2 are for the polyacetylenes alone, but are typical of a wide range of chain systems.

Polyacetylene is basically a chain $(CH)_N$ with alternating single and double bonds between carbons (—C═C—C═C—), the hydrogen saturating the fourth bond of each carbon. There are two main isomers, namely the *cis* and *trans* forms. We may concentrate on the *trans* form here (t − PA), since it shows more novel features. The defects may be classed in several ways, these describing (i) the sequence of single and double bonds and (ii) the net charge; here, for instance, • indicates an extra electron placed in an sp^3 orbital and + an electron removed from an sp^3 orbital. The *sequence of bonds* is especially significant. For *t*-PA, there are two equivalent arrangements of bonds, namely those with double bonds on the right and those with double bonds on the left; these are said to have dimerisation (or phase of opposite signs, the dimerisation at a carbon m‿asuring the difference in length of the two bonds to that carbon). If there is a localised defect in a chain produced by adding or removing electrons only, then either (i) the dimerisation changes sign across the defect (e.g. double bonds to the left on one side and to the right on the other side); in this case the defect is a species of soliton; band-gap excitation yields a pair of mobile charged solitons, S^+ and S^-; or (ii) the dimerisation does not change sign across the defect (e.g. double bonds all to the left far from the defect on either side). In this the defect is a species of polaron. Note even numbers of solitons cannot be distinguished from polaronic species with these definitions.

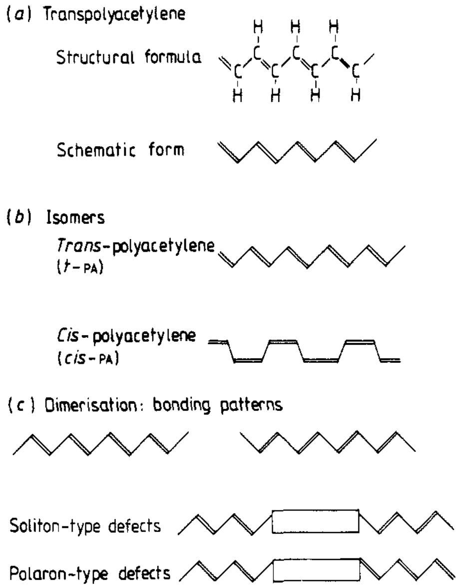

Figure 1. Polyacetylenes, showing regions of undisturbed conjugation. The boxes in (*c*) indicate a region of altered conjugation. Note that switching double and single bonds in *cis*-PA produces *inequivalent* forms, so that there is no electronic defect analogous to the soliton. Other forms of *cis*-PA exist; only the most stable is shown.

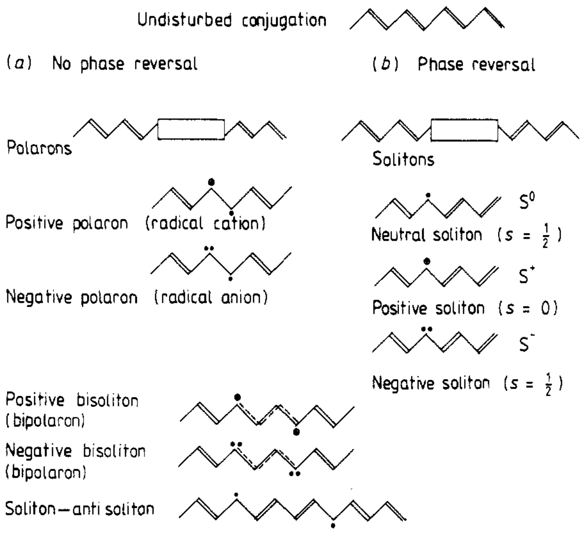

Figure 2. Defects in polyacetylenes. Here electronic defects in *t*-PA are shown, categorised by whether or not the dimerisation (phase) changes sign across the defect. The soliton–antisoliton pair is shown at the closest reasonable spacing. The extent of bonding (single versus double) is schematic, i.e. there will be a relatively smooth variation along the chain, not the abrupt form shown.

Acknowledgments

The initial stimulus for this survey arose in discussions with Professor Fritz Lüty (University of Utah, Salt Lake City) at the 1984 International Conference on Defects in Insulating Crystals.

General references and further reading

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