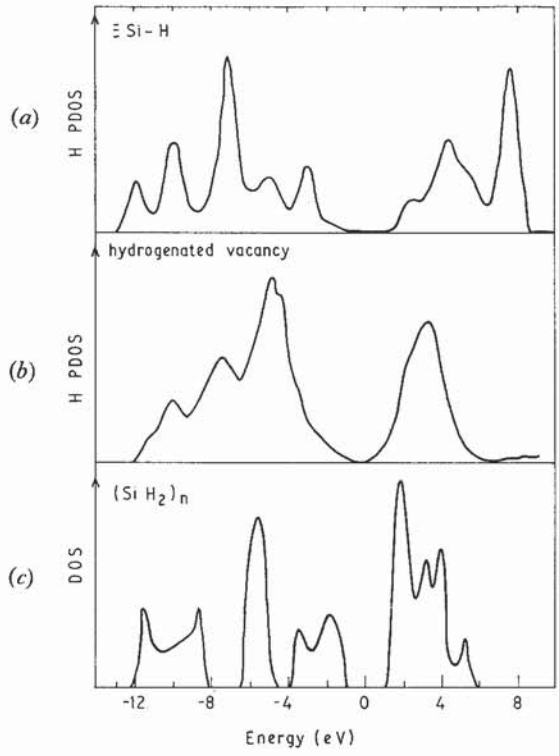
Fig. 45



LCAO DOS for: (*a*) on isolated Si–H unit after [525]; (*b*) TB DOS for the hydrogenated vacancy; and (*c*) the $(SiH_2)_n$ polymer using the Si sp^3s^*, H sp^* basis after [532].

states at −6 eV [523] and the Si–H σ^*states in the lower conduction band [522]. The calculations show that hydrogen passivates dangling bonds by converting the gap states into Si–H σ and σ^* states at −6 and 1·5 eV, respectively. H is slightly more electronegative than Si and the Si–H bond is polarized towards the H end. Calculations confirm that the gap increases due to a retreat of the *p*-like valence states, and suggest a maximum retreat of $V(pp\pi)$, or about 0·72 eV, if only ≡SiH units are present [532]. The various peaks around −6 to −8 eV in the lower valence band due to Si–H σ states have related to the underlying topology of Si lattice [528]. The Si–H σ^* states lie at the conduction band edge if the ≡SiH units are connected as sixfold rings of *trans* Si–Si bonds, but otherwise the states can lie higher into the conduction band. Interestingly, Si 2*p* yield spectroscopy finds a featureless conduction band in a-Si : H, and little trace of well-defined Si–H σ^* states [4]. Perhaps disorder broadens these σ^* states much more than the σ states.

The hydrogenated vacancy is a useful computational device in the study of a-Si : H [529–532]. The four dangling bonds of a vacancy are each saturated by H atoms, restoring their bonding and maintaining the local T_d symmetry. The ideal hydrogenated vacancy is very compact and unlikely to be found in real a-Si : H according to NMR H line-width measurements [512]. However, H is so small that the H–H interactions within the vacancy are moderate. Self-consistent pseudopotential

calculations of the local DOS and charge densities of the hydrogen vacancy show the existence of four well-defined Si–H bonds. Standard defect Green's function techniques can also be used for the hydrogen vacancy because of its T_d symmetry. Some LDF pseudopotential calculations find little erosion of the local valence band DOS at the ideal hydrogenated vacancy [530]. TB calculations do find an erosion of the local DOS [529, 532]. Presumably the conflict arises because the TB calculations are parametrized against SiH_4 and underestimate the H–H interactions across the vacancy. However, as the hydrogenated vacancy is unlikely to exist in this ideal (undistorted) form in a-Si : H, the TB results are more representative.

While the passivating behaviour of $\equiv$SiH units in a-Si : H is reasonably well understood, this is not so for $=SiH_2$ units. Polysilane or $(SiH_2)_n$ is believed to be the principal constituent of the deleterious intercolumnar phase of low density a-Si : H [509]. It is also a major constituent of high H-content HOMO–CVD a-Si : H which has a wider gap than conventional a-Si : H and can have a very high luminescence efficiency [518]. In calculations, dihydride and trihydride groups give recognizable signatures in the valence band DOS [523, 525], and cause a larger erosion of the valence band edge than monohydride groups [532]. However, some calculations show that $=SiH_2$ groups also introduce empty σ^* H-centred states in the upper gap region [525, 528], which would be difficult to reconcile with the wider gap and higher luminescence efficiency of HOMO–CVD a-Si : H. The poorer photo-electronic properties of low-density a-Si : H and the improved luminescence of high-H HOMO–CVD is attributed experimentally to their greater and lower defect densities, respectively, rather than the effects of $=SiH_2$. This is because the non-radiative combination centre in a-Si : H is generally acknowledged to be the Si dangling bond rather than the $\equiv$SiH group which gives states outside the gap. Thus, there is a problem that some calculations of $=SiH_2$ energy levels are incorrect or that the group should be a recombination centre.

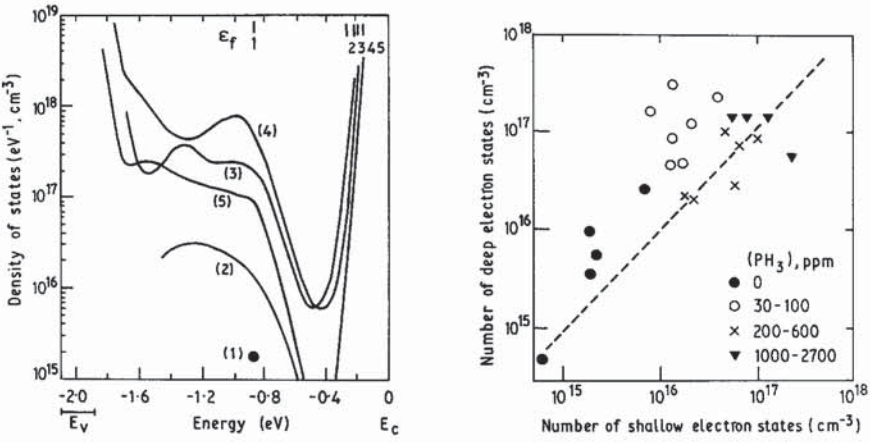
The valence band, core levels and lattice vibrations of a-Si : F have been studied experimentally [534, 535]. The electronic states have been calculated using the LCAO and TB methods [532, 536]. The Si–F bond is formed from an F $p\sigma$ state. This leaves two occupied π orbitals and one very deep s orbital on F. Although F is the most electronegative element, the Si–F bond is also strongly covalent, due to the small F radius and the $p\sigma$ character of the bond. The major signature of $\equiv$SiF units is a large peak in the valence DOS at -9 eV. F erodes the upper valence band in a similar fashion to H, experimentally and in the calculations [532, 535, 536].

8.7. *Defects in a-Si : H*

Hydrogenation leaves roughly $10^{17}\,cm^{-3}$ defects in a-Si : H. Their ESR g-value of 2·0055 is characteristic of Si dangling bonds [485, 488]. ESR, light-induced ESR, low-level light absorption and DLTS studies show that they possess a positive correlation energy of 0·4 eV, characteristic of well-localized, deep centres [488–491]. Thus hydrogenation removes all reconstructed states and leaves only a few independent Si dangling bonds.

Gap state densities ranging from 10^{15} to $10^{18}\,cm^{-3}$ have been measured by different techniques, creating a great deal of controversy. Spear and Le Comber have mapped out the entire density spectrum using the field effect on intrinsic and doped samples [25]. In contrast, DLTS finds a density dropping to less than $10^{16}\,cm^{-3}\,eV^{-1}$ at some energies (fig. 46) [487]. A probable resolution of this

Fig. 46



(*a*) (*b*)

(*a*) Energy spectrum of the gap states in a-Si : H from DLTS for films of increasing doping level (1→5) [487]. (*b*) Correlation between the total density of deep states to the number of shallow states in a-Si : H, as measured by DLTS [487].

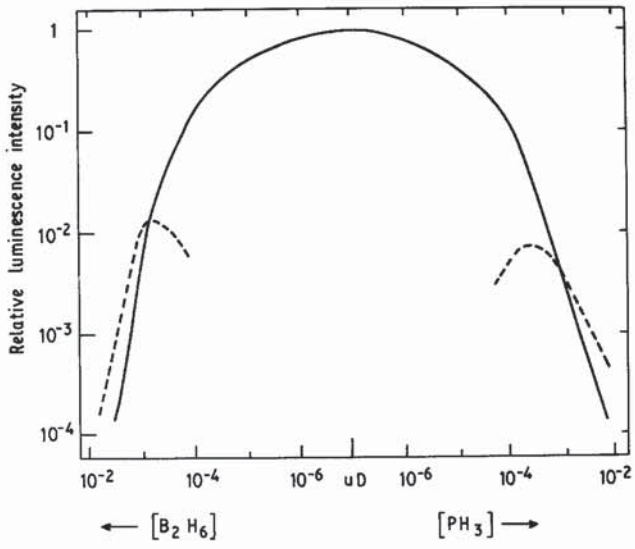
paradox is the strong thickness dependence found by low-level optical absorption, indicating a strong concentration of defects at surfaces [537]. A higher density is measured by surface-sensitive techniques like field-effect while DLTS mainly senses the bulk density. The origin of the surface enhancement of defect density is not yet understood [537] but has important implications for all thin-film devices.

The second source of the disagreement is the strong dependence of defect density on doping levels. The luminescence efficiency of a-Si : H depends largely on the defect density, as they act as non-radiative recombination centres whatever the position of ε_f [520]. The efficiency falls by a factor of 10^3 at high doping levels indicating a large increase in defect density (fig. 47). It is therefore completely incorrect to treat the defect spectrum as fixed and independent of doping level, as it is often portrayed [25]. The total density and presumably the precise spectrum are strongly dependent on the doping levels, as indicated by DLTS [487] (fig. 46). It is unfortunate that DLTS can only measure defect spectra in the more conductive doped films, from ε_f towards the gap centre, and that currently *p*-type films have been unresponsive.

The cause of the doping dependence of the defect density will be discussed shortly in §8.8. Higher doping levels increase the density of defects measured by DLTS, combined LESR/ESR studies or estimates from photoconductivity measurements [24, 487, 489, 491, 520, 538]. Compensation reduces the density towards the undoped value [520]. This indicates that their density is controlled by the position of ε_f rather than the total doping level.

The tail-state density is probed by a variety of techniques and has been interpreted variously in terms of exponential tails [491, 521, 539] or structured distributions [540]. Light-induced ESR and ESR measurements show three basic signals, that at $g = 2{\cdot}0055$ due to Si dangling bonds, $g = 2{\cdot}004$ assigned to electron tail states and $g = 2{\cdot}013$ assigned to hole tail states [485]. The doping dependences confirm these interpretations [489] but they await theoretical confirmation.

Fig. 47



Variation with doping level of the 1·35 eV luminescence in a-Si : H. The 0·9 eV defect-related luminescence is shown by the dashed lines.

8.8. *Doping of a-Si : H*

Substitutional doping of a-Si was considered unlikely for many years because it was believed that the absence of topological constraints on a CRN allowed each atom to satisfy its valence within the 8-N rule. Substitutional doping of c-Si was attributed to the large strain energy needed to include any threefold non-doping sites in a crystalline lattice. Experimentally, doping by elements of groups I, III and V is observed if the gap-state density of a-Si is sufficiently low. Group I elements are assumed to enter interstitially and group III or V elements like B or P are assumed to be substitutional. However, unlike in c-Si, substitutional sites in a-Si : H are outnumbered by the three-fold 'alloying' sites which are assumed to be electronically passive [24]. The presence of alloying sites lowers the doping efficiency in a-Si : H. Estimates of doping efficiency have fallen recently. Although this will make definite experimental verification of the substitutional mechanism difficult, it is worth noting that the observed changes in electronic properties can only be explained by sites with co-ordinations different to 8-N, such as substitutional sites. Direct evidence for substitutional sites has recently been found in NMR [541], the earlier evidence from EXAFS [542] was obscured slightly by H.

Two types of explanation have been offered to account for the presence of substitutional sites: that either finite bandwidths or defects stabilize substitutional doping. Robertson [126, 543] suggested that small numbers of sites violating the 8-N rule are allowed in the presence of finite bandwidths. Considering the case of phosphorus, P_3^0 sites are required by the 8-N rule in bulk phosphorus as this leaves all σ^* states empty. A P_4^0 would cause an electron to enter a less stable σ^* state. The energy penalty for this is reduced if the host is a-Si because the electron occupies a

more stable conduction band-edge state, rather than a pure σ^* state. Light elements were found to be more stable at substitutional sites when energies were estimated using a Weaire–Thorpe model.

In an alternative theory, Street [24] suggested that substitutional sites were stable only if ionized, with the free carrier becoming trapped elsewhere at a defect. Thus, the 8-N rule applies to the actual electronic configuration of the dopant; a neutral phosphorus with five electrons will be triply co-ordinated P_3^0, while a substitutional P atom must be positively charged to be stable, viz. P_4^+. Street then suggested that the relative concentrations of P_3^0 and P_4^+ adjust to ensure that no P_4 states become occupied—that ε_f lies below the donor band. The electrons are donated to defect states lower in the gap by the reaction

$$P_3^0 \rightarrow P_4^+ + D^-. \tag{49}$$

Charge neutrality relates the total concentrations of phosphorus, N, and the concentration of substitutional sites, n, by:

$$[P_4^+] = [D^-] = n \tag{50}$$

and

$$[P_3^0] = [P] - [P_4^+] = N - n, \tag{51}$$

and the law of mass action gives:

$$\frac{n^2}{N-n} = K, \tag{52}$$

giving a doping efficiency $\eta = n/N$ which falls as $N^{-1/2}$ for $n \ll N$:

$$\eta = n/N \simeq K^{1/2} N^{-1/2}, \tag{53}$$

which is seen experimentally [24]. The theory neatly explains the experimental absence of dopant ESR signals and inability of ε_f to approach closer than about 0·2 eV to the band edges where the forbidden P_4^0 band lies. It also explains the reduction of defect density by compensation [520]. Substitutional sites only exist in a-Si : H in the presence of an equal number of defects, according to eq. (39). The creation of more defects is consistent with the decreasing luminescence efficiency at high doping levels. Clearly this is an important technological consequence, it may be difficult to prepare films of simultaneously high conductivity and high carrier lifetimes.

Although the two theories of Street [24] and Robertson [126] have very different implications for the doping process, the source of this difference is quite subtle. In Robertson's theory the P_4 electron delocalizes away from this site into the host's band-edge states. If experiment does point to the absence of P_4^0 sites, it is remarkable that the instability of P_4^0 could be driven by such a small on-site charge density. This can only be resolved if dopant states are deep and have a sizeable on-site charge density. Then Street's proposition about co-ordinations and the 8-N rule applies specifically to deep dopant states. It can be restated thus: 'localized antibonding states cannot be occupied, nor can localized bonding states trap holes and remain stable configurations'. We must then postulate a strong electron–lattice coupling to be present at such gap states of σ or σ^* character to prevent the forbidden occupations. This forces sites producing deep states to obey the 8-N rule. An incorrect occupation causes the bond to break into dangling bonds. Dangling bonds

have $U > 0$ and are stable for all occupations in a-Si : H. Framing Street's proposition in terms of σ and σ^* states points towards a unified description of gap states in a-Si : H and a-Se within Anderson's original polaronic model [417]. The inability of a dangling bond in a-Si to overcoordinate remains as an exception, but the similarity exists between their σ and σ^*-like states. The corollary is that doping self-limits in a-Si : H because ε_f remains trapped in localized states.

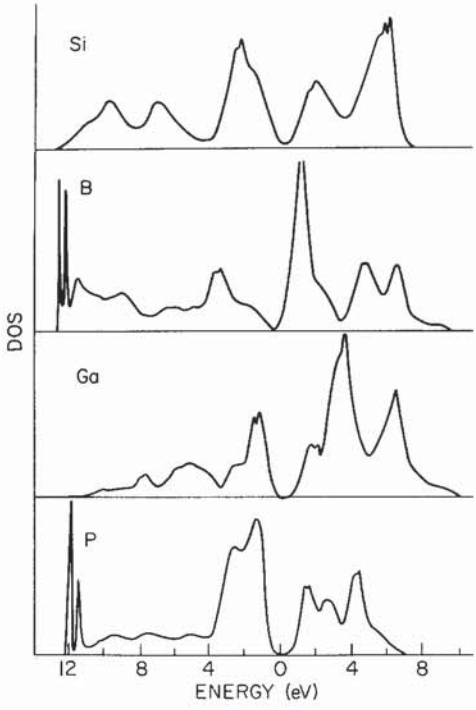
Interstitial doping can be achieved in a-Si : H by in-diffusion of alkali metal such as Li [544]. No self-limiting effect is now expected theoretically as such electropositive elements should always ionize but apparently this is found experimentally. However, this may result from diffusion, thermal stability or segregation.

A low density of gap states is a prerequisite for observable doping in a-Si. It is generally assumed that monovalent passivants such as H or F are required to reduce the defect density. However, recently, doping has been observed in CVD a-Si [545] with a very low H-content showing that passivants can be avoided. It is possible that the higher temperature deposition of CVD a-Si produces a better quality of local bonding in a-Si, a process originally suggested by Spear for the good properties of glow discharge a-Si [25]. An important aspect of CVD films is that conductivity changes occur only above a threshold doping level, showing that initially the dopants themselves compensate the remaining defect states.

The levels of alloying and substitutional sites in a-Si : H have been calculated by the tight-binding method [126, 546]. The alloying sites are assumed to have local configurations expected from the 8-N rule and are assumed to be electronically passive (§ 2.2, fig. 3). The pnictides are found to add states to the valence bands but do not produce any gap states, confirming their passivity (fig. 48). Most group III elements were found to form strong sp^2 bonds and leave an unoccupied π level well into the conduction band, again confirming their passivity. However, first row elements are often anomalous, and B is predicted to give non-bonding states near the conduction band edge or lower in the gap, depending on the site's distortion. This may account for lower doping efficiency of B than P, but the presence of B-derived gap states needs experimental confirmation [546].

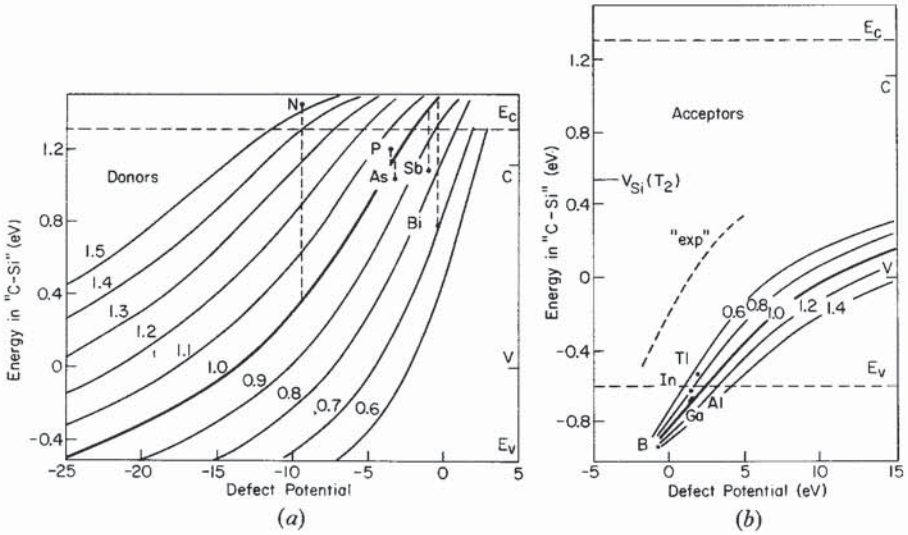
The depth of gap states due to the substitutional sites can be calculated by Green's function methods. Substitutional sites in a-Si : H differ from those in c-Si in that the absence of constraints allows the dopant atoms to adopt their normal covalent radii, rather than be forced to occupy a site of possibly very different size [126]. This change is particularly marked for the small first row elements B and N. Thus we assume that the bond lengths are the sum of the covalent radii. The dopant gap states can be shallow or deep depending on the strength of the impurity potential. There is a much greater possibility of deep states in view of the much wider gap of a-Si : H ($\simeq 1{\cdot}8$ eV) than c-Si. Energies of deep states are accurately described by a TB Green's function defect calculation with the impurity potential respresented only by its central-cell part. A deep state is found if the central-cell potential binds a state. Otherwise, the Coulombic tail binds shallow states. The central-cell potential consists of two parts, the difference in orbital energies of impurity and host, and the changes in the interactions arising from size differences. The results are conveniently plotted against orbital energy differences as a series of curves for various dopant radii to emphasize chemical trends (fig. 49). Smaller dopants and weak impurity potentials produce the most shallow levels. The curves for independent donors and acceptors show that heavier elements give deeper levels. P is interpreted as slightly deep while N is predicted to be shallow because of its small radius. B is also predicted

Fig. 48



DOS of three-fold co-ordinated P, Ga and B sites in a-Si, compared to the local Si DOS, from a TB cluster recursion calculation [546].

Fig. 49



Dopant level depths in a-Si : H for (*a*) donors and (*b*) acceptors [126]. The depths are plotted as a function of dopant orbital energy and dopant interaction. The interaction ratio R can be related to the ratio of dopant to Si atom radius by assuming a d^{-2} scaling. A deep state is found if the solution lies in the gap. If the solution lies in the bands, the dopant produces only a shallow state. The gap of a-Si : H is taken to be 1·8 eV and aligned against the valence maximum of c-Si form −0·5 eV to 1·3 eV.

to be shallow [126]. Clearly not all dopants produce deep levels, and more work is required to investigate the consequences of this for the '8-N rule' of dopant sites [24], just discussed.

The calculations were also extended to a range of distorted and hydrogenated environments. Donor states are symmetric (A_1), which are relatively insensitive to angular disorder, while acceptor states are T_2 (if deep) and strongly disorder broadened [126]. Substitutional sites with one of the four Si replaced by H are found to give equally shallow levels, in general, so H does not have a deleterious effect on dopant level depths [532].

There are a number of incompletely understood metastable effects in a-Si : H which could be associated with its defect states. The Staebler–Wronski effect [547] is a photo-induced reduction of the dark and photoconductivities of doped a-Si : H. A photo-induced creation of dangling bonds has also been observed [548]. Finally, the apparent doping efficiency in a-Si : H can be modulated by an electric field by an amount considerably greater than the base efficiency—a field-induced doping effect [549].

There has been considerable debate whether the Staebler–Wronski effect is a bulk effect in which ε_f is forced closer to mid-gap [550–553] or is a surface effect associated with band-bending, a 'thickness-dependent conductivity' [554, 555]. A photo-induced change in the bulk density of gap states was recently measured by DLTS and argues in favour of a bulk effect [556]. The influence of surfaces via an enhanced defect density rather than band-bending is becoming appreciated [537].

Street [24] pointed out that as the stability of substitutional dopant sites depends on the position of ε_f this could account for many metastable effects in a-Si : H. By expressing this stability in terms of localized or deep states, we can relate the metastabilities to changes in deep state occupancies. Broadening such a theory beyond a-Si : H could allow it to treat related photostructural changes in chalcogenides [316]. Thus, we expect electron trapping at localized σ^* gap states and hole trapping at localized σ gap states to result in bond breakage in all amorphous semiconductors.

8.9. *Defects in a-$GeSe_2$ and a-GaAs compared*

Chemically ordered covalent compound glasses contain only heteropolar bonds so the homopolar bond must be considered as a defect in addition to the dangling bond. Two situations must be distinguished: that in which each element by itself exerts its normal 8-N co-ordination, as in a-$GeSe_2$ and a-SiO_2, and other cases such as a-GaAs where the 8-N rule applies to the pair of elements. We shall now argue that homopolar or 'wrong' bonds are more common in the former class, but dangling bonds are more common in the latter when the site regains its favoured valence.

The presence of homopolar bonds or 'broken chemical ordering' has been intensively studied recently in a-$GeSe_2$ using Mossbauer and Raman spectroscopy [40, 300, 301]. If such glasses obeyed a homogeneous random network model, the proportions of each type of bond and dangling bond could be calculated using probabilities and bond enthalpies. However, currently broken chemical ordering is being used as evidence of intermediate-range order and inhomogeneous networks in these systems. The homopolar bonds are suggested to form 'outriggers' on raft-like segments of the network, thereby reducing its overall connectivity [40, 300].

Dangling bond defects have also been studied in a-Ge_xSe_{1-x} alloys and have VAP-like character [557].

Wrong bonds have been suggested as common defects in amorphous III–V semiconductors, but experimental searches have been inconclusive (see §7·5). Dangling bonds were originally believed to be less stable defects, as in a-Si. However, if the surfaces of c-Si and c-GaAs are used as analogies, these suggest that three-fold Ga and As sites are more stable because of their relaxation. The surfaces of c-Si reconstruct in an attempt to expel surface states from the gap. The π bonded model of (111)Si and the asymmetrical dimer model of (100)Si both contain odd-membered rings of bonds [497, 501].

The neutral (110) surfaces of c-GaAs is its natural cleavage plane and acts as a starting model of the internal surfaces of a-GaAs, as did the (111) surface in Si. The (110)GaAs surface one dangling bond per site and it undergoes a torsional relaxation in which Ga moves in and As out, towards their natural sp^2 and p^3 configurations [558–561]. It is possible that Si-like reconstructions do not occur in GaAs because their odd-membered rings would require homopolar bonds [498]. One should also note that the relaxation of (110)GaAs is more successful than the reconstructions of Si in that no surface states remain in the gap [502, 503, 561]. Thus, Ga and As are stable in their trivalent form on this surface. The greater stability of antisites than vacancies in c-GaAs remains as evidence in favour of wrong bonds. However, we note that if the atoms around the vacancy attempt to relax towards their preferred bond angle this is opposed by the strong bond-stretching forces. Thus, the restricted relaxation at vacancies favours homopolar-bonded defects only in c-GaAs.

Acknowledgments

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Note added in proof.—The presence of intermediate range-order in silicate glasses is attracting attention recently [562–565]. Phillips has extended his cluster model [40] to SiO_2 suggesting 30 Å clusters bordered by ≡Si–O units [565]. This maintains chemical stoichiometry within each cluster, unlike this outrigger-raft model of a-$GeSe_2$ [300], but conflicts with an unstated principle of bonding of amorphous phases, that a bonding configuration, however unusual, should be found in some crystalline system.

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