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Photoluminescence Study of II-VI Semiconductors by Using Radioactive ^{71}As Dopants

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Abstract

By means of radioactive dopants, photoluminescence signals related to the respective chemical element are identified. In the present work, the isotope ^{71}As ($t_{1/2}$ = 65.3 h) which decays to ^{71}Ge ($t_{1/2}$ = 11.2 d) and subsequently to ^{71}Ga was implanted into CdTe and ZnSe. In CdTe, the (D, A) transition related to the As_{Te} acceptor is identified in agreement with the literature. In addition, a new (D, A) transition caused by a shallow Ga acceptor is identified. The corresponding acceptor level having an ionisation energy of E_i = 42 meV is still shallower than the effective-mass like state (E_i = 57 meV). It is interpreted in terms of a $^{71}Ga_{Te}$ "antisite" defect in a Jahn-Teller distorted configuration. *Ab initio* calculations within the framework of density functional theory confirm the existence of a Jahn-Teller relaxed stable configuration for Ga_{Te}. In ZnSe, no clear evidence of a (D, A_{As}) transition is found, but like in CdTe, a new shallow acceptor is observed which is supposed to originate from a $^{71}Ga_{Se}$ defect.

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I. INTRODUCTION

The optical and electrical properties of semiconducting materials crucially depend on the presence of impurity atoms, but the assignment of specific parameters – e.g. ionisation energies or exciton binding energies – to the responsible impurity atoms is often ambiguous. Backdoping experiments suffer from the possibility of the creation of intrinsic defects and defect complexes during the doping process. In order to overcome this problem, radioactive atoms are employed [1]. By recording photoluminescence (PL) spectra repeatedly after the implantation of a radioactive isotope, the change in intensity of related PL signals is determined as a function of time. If indirect effects, which can be present at high dopant concentrations [1, 2], are not dominant, the PL intensity is proportional to the dopant concentration, which changes according to the radioactive decay. Thereby, the chemical identity of the dopant causing the PL signal is revealed.

In order to get information complementary to the experimental results, calculations in the framework of the density functional theory (DFT) are performed. The DFT formalism provides a helpful tool to characterise dopants in semiconductors as well as defects and defect complexes. In the present work, such calculations are performed by means of the linearised augmented plane wave (LAPW) method, implemented in the program WIEN97 [3]. The calculations yield valuable information about the electronic properties and the local structure of the investigated defects. As shown, for example, by the success in calculating the electric field gradients caused by group V acceptors in CdTe, the calculated charge density and structural relaxation is very accurate [4].

II. EXPERIMENTAL

Bridgman-grown, nominally undoped CdTe and ZnSe crystals were implanted with radioactive ^{71}As ions provided by the ISOLDE mass separator at CERN (Geneva, CH) with a dose of 10^{13} cm^{-2} and a kinetic energy of 60 keV, resulting in an implantation depth of 30 nm. The nuclide ^{71}As decays with a half-life $t_{1/2}$ = 65.3 h to ^{71}Ge and subsequently with $t_{1/2}$ = 11.2 d [9] to ^{71}Ga. About 65h after the implantation, the samples the following discussion refers to were annealed for 30 minutes at 700 K (CdTe) and 920 K (ZnSe). In order to support the incorporation of ^{71}As at Te and Se sites, the annealing took place under Cd and Zn vapour pressure, respectively. As a reference, additional ^{71}As implanted samples were annealed under different conditions (CdTe: vacuum; ZnSe: vacuum and Se vapour). For the subsequent PL measurements the 351.1 nm line of an Ar laser was attenuated to 1.5 mW and focused to a diameter of about 200 µm on the samples, which were cooled down to 1.6 K. The luminescence was analysed by a 0.5 m grating monochromator and detected by a CCD camera. Between the different PL measurements, the temperature of the samples was hold below 150 K in order to avoid modifications of the samples originating from processes other than the radioactive decay. In PL experiments, it is generally difficult to reproduce absolute intensities exactly, therefore PL lines related to radioactive dopants are usually normalised to lines which are known to be caused by stable elements [1].

III. RESULTS AND DISCUSSION

A. The ^{71}As acceptor in CdTe

Figure 1 shows a subset of the PL spectra of the ^{71}As doped CdTe sample recorded after the annealing process. At the beginning of the sequence, the PL line at 819 nm is the dominant feature in the spectrum at the low energy side of the excitonic region. This line was already attributed to the recombination of electrons bound to effective-mass like donors (ionisation energy $E_i \approx 14$ meV) with holes bound to As acceptors [(D, A_{As}) transition] [5]. The spectra also show the phonon replicas of this zero-phonon-line (ZPL) which are separated by the LO-phonon energy of 21.2 meV from each other. Both the position of the (D, A_{As}) transition as well as the phonon coupling constant are in agreement with the data from Ref. [5]. Normalised to the (D, A) transition at 804 nm, which is generally attributed to Li and Na acceptors [6], the time dependence of the intensity of the ZPL at 819 nm follows directly the radioactive decay of ^{71}As: A fit to the PL intensity $I(t)$ using

$$I(t) = Ae^{-t/\tau} + B \qquad (1)$$

yields a half-life of $t_{1/2}$ = 65(3) h ($t_{1/2} = \ln 2 \cdot \tau$), in excellent agreement with the half-life of ^{71}As (cf. Figure 2a; the time t is defined as the time after the annealing process). Thereby, the line at 819 nm is unambiguously assigned to As acceptors, and the identification in Ref. [5] is confirmed. It should be noted that in the reference sample annealed in vacuum this signal is absent, revealing the sensitivity of the incorporation of As as acceptor at the Te site on the annealing conditions.

B. The ^{71}Ga acceptor in CdTe

The concentration of Ga atoms created by the radioactive transmutation $^{71}As \rightarrow ^{71}Ge \rightarrow ^{71}Ga$ is given by the expression

$$c_{Ga}(t) = c_0\left(1 - \frac{e^{-(t-t_0)/\tau_{Ge}}}{1-\tau_{As}/\tau_{Ge}} - \frac{e^{-(t-t_0)/\tau_{As}}}{1-\tau_{Ge}/\tau_{As}}\right), \quad (2)$$

which can be calculated from the decay laws. Equation (2) describes the total Ga concentration, if c_0 is set to the total concentration of implanted ^{71}As ions and t_0 is set to the implantation time. During the sequence of PL measurements, a new PL line appears at 794 nm (cf. Figure 1), and increases steadily until it saturates after about 500 h. The time dependence of this signal is obviously strongly correlated with the concentration of ^{71}Ga atoms. In Figure 2b, the PL intensity is compared to the Ga concentration according to equation (2), where an appropriate constant has been added in order to account for the background in the PL signal, and a suitable value for c_0 has been chosen (the freedom for this parameter accounts for the – not explicitly known – factor of proportionality between the concentration and the PL intensity). Furthermore, t_0 has been set to the annealing time (i.e. $t_0 = 0$ according to the definition of t) instead of the implantation time ($t_{impl.} = -65$ h, left margin of Figure 2b), indicating that not the total Ga concentration contributes to the PL intensity, but only a part (the role of t_0 is discussed below in detail). By the convincing qualitative relation between the PL intensity and the Ga concentration, the PL line at 794 nm is unambiguously attributed to Ga atoms.

For $t > 400$ h, the intensity follows no longer the Ga concentration. This saturation behaviour can, at least partly, be explained by an indirect process (i.e. a process not directly related to the change in concentration): Possibly due to the creation of additional nonradiative centres along with the radioactive decay, even the intensity of lines caused by stable impurities, e.g. the (D, $A_{Li, Na}$) transition, is dropping by a factor of 3 until the end of the sequence. The Ga related line is more sensitive to the loss of effective excitation power than the (D, $A_{Li, Na}$) transition to which it is normalised, and therefore it is subject to an apparent decrease of intensity.

Figure 3 shows that the Ga related PL line at 794 nm vanishes at a sample temperature of about 30 K and that it is replaced by a new line at 792 nm. This behaviour is interpreted as the typical transformation of a (D, A) transition into a free-electron to acceptor transition [(e, A) transition] at the temperature where the effective-mass like donors become ionised. Accordingly, the line at 794 nm corresponds to a (D, A_{Ga}) transition involving the Ga atom as an acceptor. This is a surprising observation because Ga is normally incorporated as a donor at a Cd site [7]. From the (e, A) transition, the ionisation energy E_i of the acceptor state can quite accurately be determined using [8]:

$$E_i = E_g(T) - E_{ph} + \tfrac{1}{2}kT \quad (3)$$

Here, E_{ph} is the photon energy and $E_g(T)$ is the temperature dependent gap energy which is taken from Ref. [7]. Thus, the ionisation energy of the Ga acceptor is determined to $E_i = 42(1)$ meV, which is considerably smaller than the energy of an effective-mass like acceptor ($E_i = 57$ meV [7]). The low ionisation energy is remarkable, since all known substitutional acceptors in CdTe have effective-mass like energies or, due to central-cell corrections, higher ionisation energies than effective mass-like acceptors [7]. In a similar way, the ionisation energy of the As_{Te} acceptor has been determined to $E_i = 92(1)$ meV, which is in agreement with Ref. [5].

Since the presence of As_{Te} acceptors in CdTe is confirmed by the (D, A_{As}) transition observed at the beginning of the sequence, the creation of Ga_{Te} 'antisite' configurations by the radioactive transmutation is expected (here, the term 'antisite' is used in contrast to the above mentioned 'normal' incorporation of Ga at a Cd site). Thus, the radioactive transmutation process leads to a specific defect configuration that is different from the equilibrium configuration. It should be remarked that the recoil energy up to 26 eV [9] disposed on the ^{71}Ge daughter nucleus due to the decay of ^{71}As can affect the lattice location of a part of the ^{71}Ge atoms. Furthermore, not all of the ^{71}As atoms might be incorporated initially at a Te site. Consequently, not necessarily all ^{71}Ga atoms will finally be left as Ga_{Te} antisites, but this configuration is the most obvious candidate for the observed Ga acceptor.

Within the time span of 65 h between the implantation and the annealing process, already half the ^{71}As atoms have been decayed to ^{71}Ge and also a small fraction of ^{71}Ga atoms has been created. Therefore, the annealing behaviour of all three elements influences the population of Ga_{Te} configurations. The incorporation of As at the Te site after the annealing under Cd vapour pressure is evident by the observation of As_{Te} acceptors (see previous section). Additional information about the annealing behaviour of Ge and Ga in CdTe can be achieved by an analysis of the exact shape of the curve describing the intensity of the (D, A_{Ga}) transition as a function of time: First, the intensity just after the annealing is close to zero (cf. Figure 1 and Figure 2b at $t = 0$), accounting rather for a background than for a contribution by the ^{71}Ga atoms that have been created between the implantation and the annealing. Obviously, the Ga atoms which are already present at the annealing time do not

contribute to the (D, A_{Ga}) transition. According to the normal behaviour of Ga in CdTe these atoms are probably incorporated as donors at Cd sites by the annealing process and thus do not contribute to the concentration of Ga_{Te} antisite configurations. Second, the curve starts with a zero slope (cf. Figure 2b), indicating that the ^{71}Ge atoms are not incorporated at the Te site during the annealing. If they would occupy the Te site, they would populate the Ga antisite configuration by the decay $^{71}Ge_{Te} \rightarrow {}^{71}Ga_{Te}$ immediately after the annealing and cause a positive slope. The annealing behaviour of Ge is also the reason why equation (2) describes the time dependence of the (D, A_{Ga}) transition properly only if t_0 is set to the annealing time instead of the implantation time (cf. Figure 2b): Since both Ge and Ga are not incorporated at the Te site, the population of Ga_{Te} via the decay $^{71}As_{Te} \rightarrow {}^{71}Ge_{Te} \rightarrow {}^{71}Ga_{Te}$ is resetted at the annealing time and the population starts from the beginning with the decay of $^{71}As_{Te}$. It should be noted, that the conclusion about the annealing behaviour of Ge is also in agreement with the fact that the observation of Ge atoms as double donors at Cd sites has been reported [10], while the observation of the expected double acceptor character of Ge at Te sites has been lacking [7]. Thus, the interpretation about the annealing behaviour of Ge and Ga and the assumption that Ga_{Te} antisites form the new Ga acceptor yield a fully consistent picture. A further confirmation that Ga antisites are observed is delivered by the vacuum annealed sample: There, no As_{Te} acceptors are detectable; the Ga_{Te} configuration is consequently not populated and also the (D, A_{Ga}) transition is not observed.

C. ^{71}As doped ZnSe

In contrast to CdTe, there is no clear evidence of a (D, A_{As}) transition in ZnSe after implantation of ^{71}As and subsequent annealing. Shallow levels (E_i = 110 meV and E_i = 60 meV), arising from As doping are reported in the literature [11], but are not observed in the present experiment. There is a (D, A) transition observed [Figure 4, labelled (D, A_{EM})], involving an effective-mass like acceptor with an ionisation energy of E_i = 109(1) meV, but this line is obviously caused by a stable species: The intensity decreases not more than the overall intensity of the spectrum, which, similar as in CdTe, decreases by about a factor of two during the sequence. The absence of PL lines involving As acceptors seems to be a consequence of the general difficulty to achieve p-type conductivity in ZnSe. On the other hand, it is obvious that the compensation of As acceptors is not caused just by the formation of – isolated – compensating donors, since in this case, a (D, A_{As}) transition should be observed. A possible reason for the lack of such a transition might be that the ^{71}As atoms are not incorporated properly at substitutional Se sites, or that they form complexes during the annealing process that are electrically inactive.

Within the first days of the sequence, a new (D, A) transition at 452 nm appears which essentially stays at a constant intensity after 5 days (see Figure 4). Since this line is not decreasing again, it is assigned to a Ga defect. Similar as in CdTe, this Ga related line corresponds to an acceptor that is shallower than the effective-mass like acceptor. A clear shift from a (D, A_{Ga}) to a (*e*, A_{Ga}) transition is not observed as it is in CdTe. This fact might be caused by the specific value of the Coulomb term that enters the energy of the (D, A) transition: If this term has about the value of the donor ionisation energy, both transitions have about the same energy and the shift is not observable. Assuming the (*e*, A) transition to dominate at T_M = 49 K, the ionisation energy E_i = 73(1) meV of this acceptor is calculated using equation (3).

Due to the similar characteristics of the Ga acceptor in ZnSe compared with the Ga_{Te} acceptor in CdTe (both are shallower than the respective effective-mass like acceptor), it is supposed to originate from an analogous defect, i.e. a Ga_{Se} configuration. Since an As_{Se} acceptor is not observed, the population of the Ga_{Se} configuration is in question and an analysis of the time dependence of the PL intensity – similar as in CdTe – is made: The time dependence of the (D, A_{Ga}) transition shows up a more pronounced saturation behaviour compared to CdTe, but also has an important difference just after time zero: The curve starts with a non-zero slope (see Figure 5), showing that the ^{71}Ge atoms, which have been created between the implantation and the annealing time, do contribute to the (D, A_{Ga}) transition – in contrast to the observation in CdTe. Therefore, the population of the Ga_{Se} configuration is explained by the incorporation of Ge at Se sites at the annealing time and the subsequent decay $^{71}Ge_{Se} \rightarrow {}^{71}Ga_{Se}$. The reference samples which are annealed in vacuum and under Se vapour pressure, do not show up the (D, A_{Ga}) transition, thereby giving the indication that Ge is incorporated at the Se site only if the annealing takes place under Zn vapour pressure. If the PL intensity of the $^{71}Ga_{Se}$ line is governed only by the decay of the $^{71}Ge_{Se}$ atoms, the Ga concentration which contributes to the intensity of the (D, A_{Ga}) transition is given by:

$$c_{Ga}(t) = c_0\left(1 - e^{-(t-t_0)/\tau_{Ge}}\right). \qquad (4)$$

Here, c_0 corresponds to the concentration of Ge atoms that are incorporated at Se sites by the annealing process and t_0 corresponds to the annealing time. A different time dependence is expected, if the transmutation $^{71}As \rightarrow {}^{71}Ge \rightarrow {}^{71}Ga$ of ^{71}As atoms decaying after the annealing would contribute besides the transmutation $^{71}Ge_{Se} \rightarrow {}^{71}Ga_{Se}$ to the intensity of the (D, A_{Ga}) transition. In this case, the PL intensity would follow the Ga concentration given by equation (2), with t_0 accounting now for the implantation time. This, however, should not

be the case, because the absence of a PL signal arising from As_{Se} acceptors implies that the Ga_{Se} configuration should not be populated by the decay $^{71}As \rightarrow ^{71}Ge \rightarrow ^{71}Ga$.

Figure 5 shows the time dependence (D, A_{Ga}) transition. Similar as in CdTe, the intensity at $t = 0$ accounts for a background, indicating that the ^{71}Ga atoms are not incorporated at Se sites by the annealing process. Additionally, the Ga concentration according to equation (2) and to equation (4) is plotted in Figure 5. The choice of appropriate constants accounting for the background and the concentration c_0 is according to the discussion for CdTe. It should be noted that neither equation (2) nor equation (4) can account for the saturation behaviour. Despite this uncertainty, the time dependence according to equation (4) is in favour, confirming the expectation that only the Ge atoms at Se sites contribute to the final Ga_{Se} state. In the context of the lacking (D, A_{As}) transition, as discussed above, it is concluded that most of the As dopants are not properly incorporated at Se sites during the annealing (as would be expected from valence arguments) or that the As_{Se} dopants form complexes being electrically inactive. In this case, also the Ga atoms populated by the decay $^{71}As \rightarrow ^{71}Ge \rightarrow ^{71}Ga$ after the annealing would be complexed and would not contribute to the (D, A_{Ga}) transition, what is in agreement with the experimental observation.

D. Theoretical description of the Ga acceptor

In CdTe and ZnSe, which both crystallise in the zinc-blende structure, from valence arguments the Ga_{Te} and the Ga_{Se} configurations are expected to form triple acceptors (the following discussion is exemplified for CdTe, but holds for ZnSe as well). In terms of electron orbitals in a crystal field, the chemical bonds of the Ga_{Te} antisite in the neutral state are formed by a lower a_1 (s-like) state, fully occupied with two electrons, and a t_2 (p-like) state, which can take up six electrons, but is only occupied with three electrons and accommodates the three holes. Due to the presence of a degenerated, partly occupied state, the Ga_{Te} configuration can generally be subject to a Jahn-Teller distortion with C_{3v} symmetry (see Figure 6a). In this case, the t_2 level splits into an e (p_{xy}-like) state, occupied with three out of four possible electrons, and into an unoccupied upper a_1 (p_z-like) state (Figure 6b [12]). At the same time a symmetry lowering from tetrahedral to trigonal occurs. In more chemical terms, this would account for the breaking of one bond (along the *z*-direction) and a transition from sp^3 hybridisation into sp^2 hybridisation leaving an unoccupied p_z orbital. In the neutral state $Ga_{Te}^{\ 0}$, the energetically lowered e state contains a hole, whereas the full occupation of the e state corresponds to the negative $Ga_{Te}^{\ -}$ state. The doubly and the threefold negative states correspond to the occupation of the upper a_1 state which is shifted towards higher energies (cf. Figure 6b). Therefore, the experimentally observed shallow state is assigned to the $Ga_{Te}^{\ 0/-}$ level.

In order to get more detailed information than presented by this simple model, *ab initio* calculations employing the full potential LAPW method within the framework of the DFT were performed for the Ga_{Te} antisite configuration in CdTe by means of the program WIEN97 [3]. Exchange and correlation effects are treated according to the generalised gradient approximation, described by Ref. [13], and a supercell containing 32 atoms is used. Spin-orbit (SO) coupling is taken into account for the core states, but not for the valence states. Imposing the C_{3v} symmetry on the Ga_{Te} antisite, a stable configuration is found by the condition of vanishing forces, in which the Cd neighbour located in *z* direction with respect to the Ga atom has a distance of 3.3 Å, while the Cd neighbours in the *xy*-plane have a distance of 2.6 Å (see Figure 6a). All atomic positions that are shown in Figure 6a have been included into the relaxation procedure. In the LAPW method, the angular momentum character of the wavefunctions inside the atomic spheres is directly obtained. Thus, the total density of states (DOS) can be decomposed into contributions from the different angular momenta with respect to the atomic sites. Figure 7 shows the total DOS is along with the local DOS at the Ga site, decomposed into s, p_{xy}, and p_z contributions. In this way, the s-like lower a_1 level, the p_{xy}-like e level and the p_z-like upper a_1 level introduced before (see Figure 6b) are identified. Remarkably, the p_z-like upper a_1 level corresponding to the elongated, unoccupied bond is still hybridised: There are considerable s- and p-like contributions to this state at the more distant Cd neighbour in *z*-direction.

As plotted in Figure 7, the DOS does not seem to be consistent with the presence of a shallow acceptor: the e level, containing the hole (unshaded area of the e level), is about 0.6 eV above the valence band. However, the used 32 atom supercell is much too small to describe properly the extended nature of such a shallow acceptor state. This nature is reflected by the result that the e level is not strongly localised at the Ga atom, but has considerable contributions at Te atoms of more distant shells. As a consequence, the interaction between Ga impurities of neighbouring supercells still play an important role at the present cellsize, and the overlap of the impurity wavefunctions may well be responsible for the shift towards higher energies. Therefore, the data shown in Figure 7 give a basis for a more qualitative than quantitative discussion. Calculations using a bigger supercell and including SO coupling also for the valence states are planned for a further investigation, but the present, more qualitative results reproduce already nicely the Jahn-Teller distortion along with the accompanied level splitting.

IV. SUMMARY

In CdTe, the (D, A) transition and the acceptor level attributed to As acceptors in the literature are confirmed by means of PL experiments employing radioactive ^{71}As dopants. In ZnSe, no PL signal arising from ^{71}As acceptors is observed. The absence of a (D, A_{As}) transition in ZnSe is attributed to the formation of complexes involving As_{Se} acceptors or the incorporation of As at other than Se sites. Both in CdTe and in ZnSe, a (D, A) transition caused by shallow ^{71}Ga acceptors created during the radioactive transmutation is observed. This surprising behaviour of Ga is interpreted as a consequence of the creation of Ga_{Te} and Ga_{Se} antisite configurations. By an analysis of the time dependence of the Ga related PL lines, conclusions about the annealing behaviour of Ge in CdTe and in ZnSe are gained. The acceptor character of the Ga antisite configuration is discussed in terms of a Jahn-Teller distortion, which is predicted by a simple electronic model. For CdTe, the existence of a relaxed Ga_{Te} configuration in C_{3v} symmetry is confirmed by means of *ab initio* LAPW calculations.

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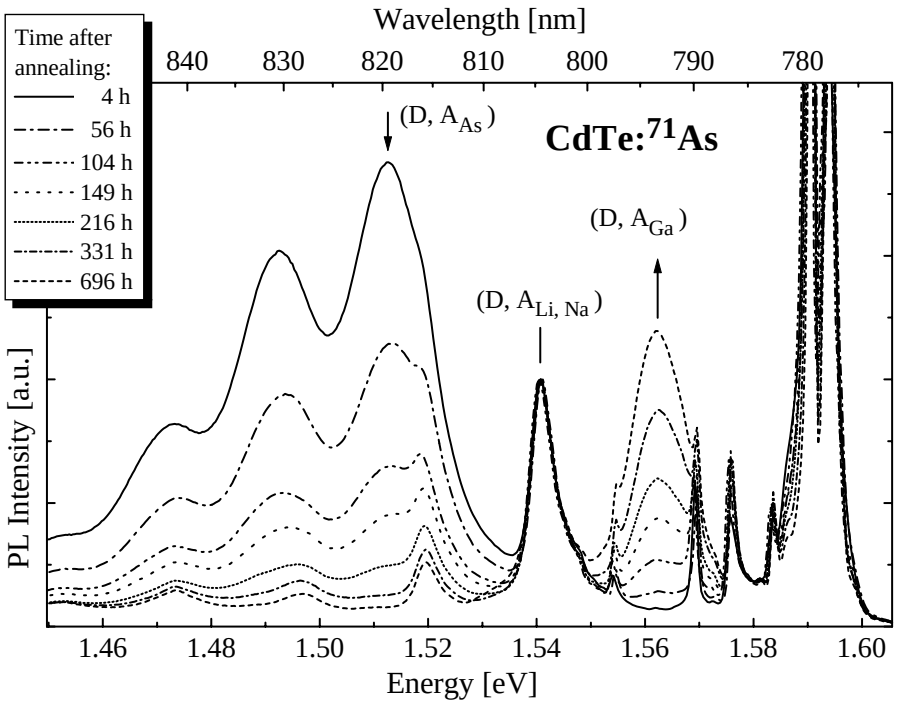

FIG. 1. A subset of the PL spectra of ^{71}As doped CdTe recorded as a function of time after annealing. The spectra are normalised to the (D, $A_{Li, Na}$) transition.

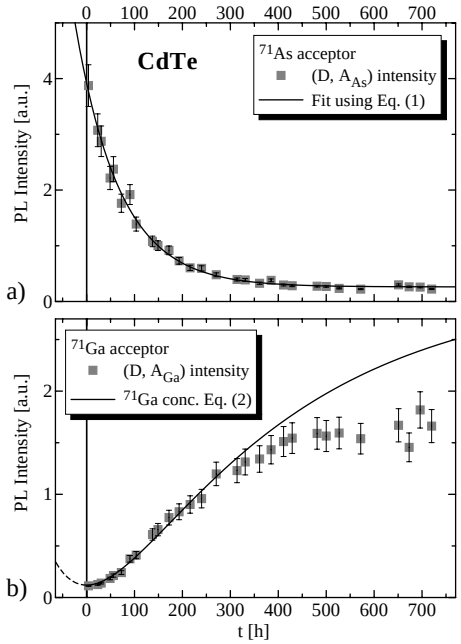

FIG. 2. (a) PL intensity of the (D, A_{As}) transition in CdTe as a function of time along with an exponential fit according to equation (1). (b) PL intensity of the new (D, A_{Ga}) transition in CdTe and the concentration of ^{71}Ga atoms according to equation (2) as a function of time. Note, that $t = 0$ marks the time of the annealing process, that $t = -65$ h (left margin) marks the implantation time, and that $t_0 = 0$ is used in equation (2).

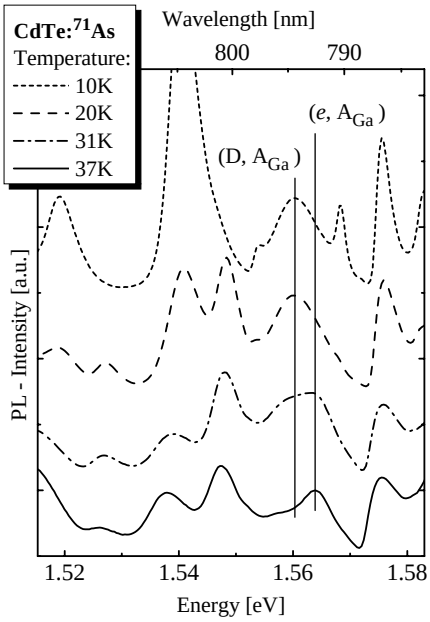

FIG. 3. Temperature dependence of the (D, A_{Ga}) transition in CdTe, showing the transformation into a (*e*, A_{Ga}) transition.

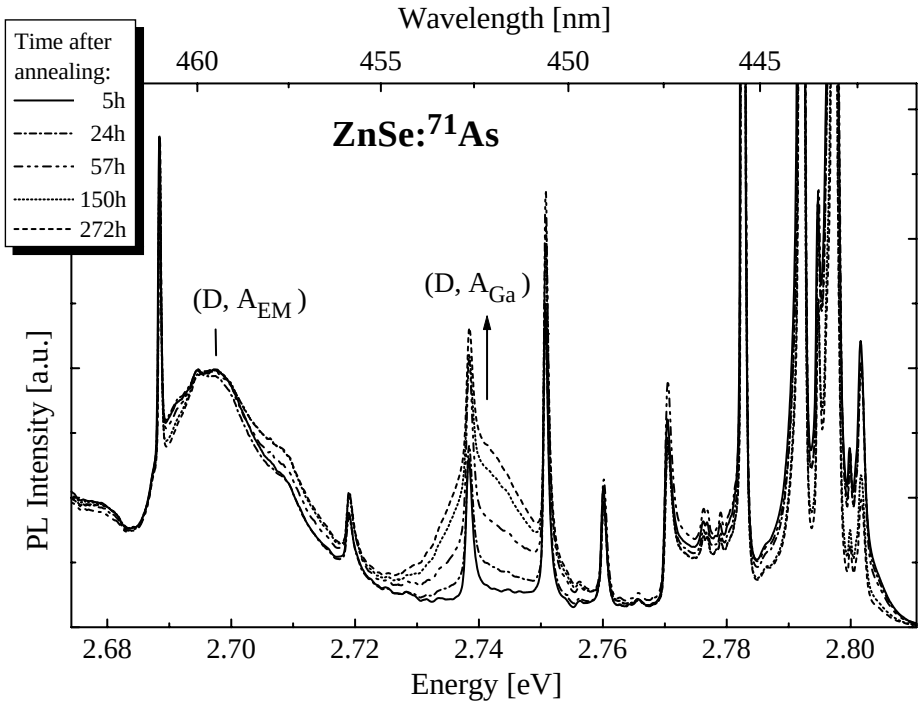

FIG. 4. A subset of the PL spectra of ^{71}As doped ZnSe recorded as a function of time after annealing. The spectra are normalised to the (D, A_{EM}) transition (A_{EM} denotes an effective-mass like acceptor).

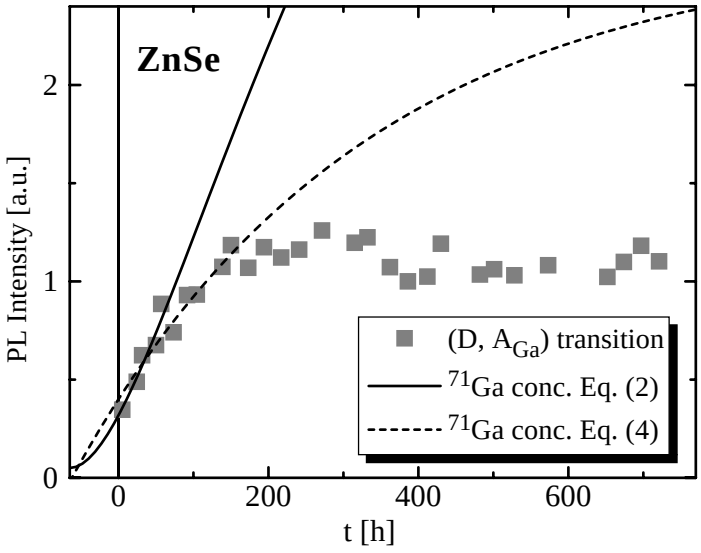

FIG. 5. PL intensity of the (D, A_{Ga}) transition in ZnSe and the concentration of ^{71}Ga atoms according to equation (2) and equation (4). Note, that $t_0 = -65$ h and $t_0 = 0$ are used in equation (2) and equation (4), respectively.

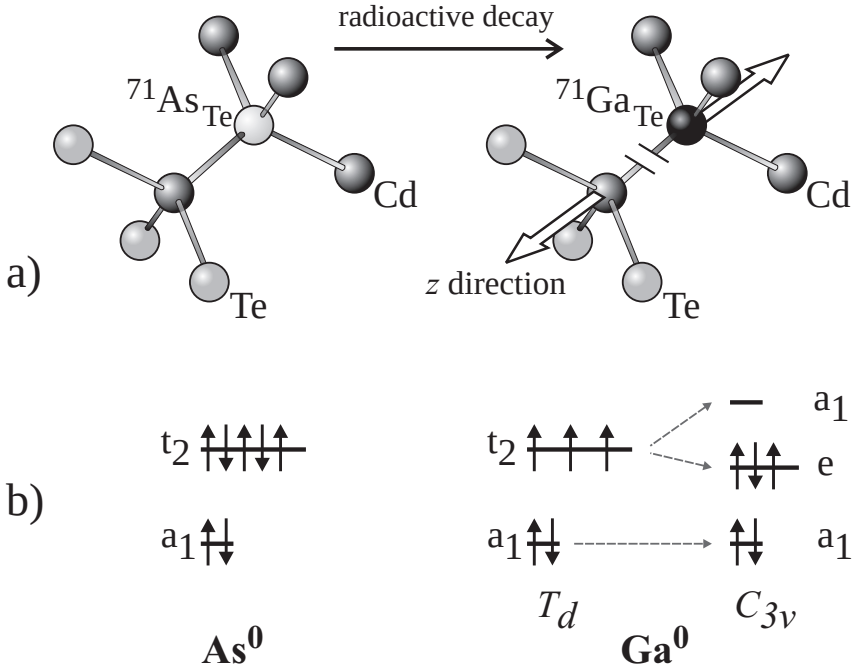

FIG. 6. (a) Schematic configuration of $^{71}As_{Te}$ in CdTe, exhibiting T_d symmetry (left), and, following the radioactive transmutation, the configuration of ^{71}Ga, exhibiting C_{3v} symmetry (right). (b) Electronic level scheme for $^{71}As_{Te}$ in T_d symmetry and for $^{71}Ga_{Te}$ in T_d and C_{3v} symmetry.

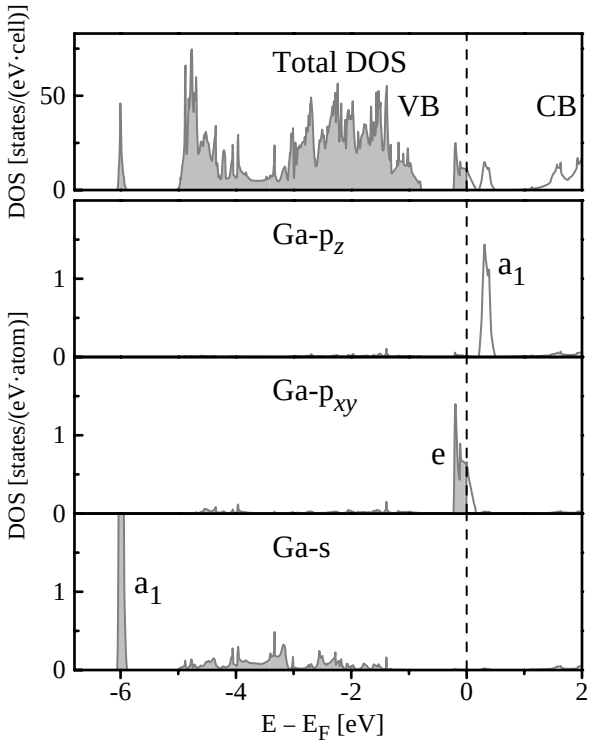

FIG. 7. Density of states for the Ga_{Te} configuration in CdTe: Total DOS (top panel) and local DOS at the Ga site, decomposed into s, p_{xy} and p_z contributions (bottom panels).