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Positron-lifetime study of compensation defects in undoped semi-insulating InP

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Positron-lifetime and infrared-absorption spectroscopies have been used to investigate the compensation defects that render undoped *n*-type liquid encapsulated Czochralski-grown InP semi-insulating under high-temperature annealing. The positron measurements, carried out over the temperature range of 25–300 K, reveal in the as-grown material a positron lifetime of 282 ± 5 ps which we associate with either the isolated indium vacancy V_{In}^{3-} or related hydrogen complexes. The shallow donor complex $V_{\mathrm{In}}\mathrm{H}_4$, responsible for much of the *n*-type conductivity and the strong infrared absorption signal at 4320 nm, is ruled out as a significant trapping site on the grounds that its neutral state is present at too low a concentration. After annealing at 950 °C, in conjunction with the disappearance of the $V_{\mathrm{In}}\mathrm{H}_4$ infrared-absorption signal, trapping into V_{In}-related centers is observed to increase slightly, and an additional positron trapping defect having a lifetime of 330 ps appears at a concentration of $\sim 10^{16}$ cm^{-3}, indicating divacancy trapping. These results support the recent suggestion that the $V_{\mathrm{In}}\mathrm{H}_4$ complex present in as-grown InP dissociates during annealing, forming $V_{\mathrm{In}}\mathrm{H}_n^{(3-n)-}(0\leqslant n\leqslant 3)$ complexes and that the recombination of V_{In} with a phosphorus atom results in the formation of EL2-like deep donor P_{In} antisite defect, which compensates the material. It is suggested that the divacancy formed on annealing is $V_{\mathrm{In}}V_{\mathrm{P}}$, and that this defect is probably a by-product of the P_{In} antisite formation.
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I. INTRODUCTION

In recent years, InP has been considered a potentially important material for the development of optoelectronic devices. Such devices often require InP in semi-insulating (SI) form as a substrate material. Until recently the only method of forming SI-InP has been through Fe doping, in which deep acceptors compensate for the residual free electrons that are present even in the purest undoped as-grown substrates. However, the presence of the Fe dopant often affects device performance.[1,2] The discovery that a semi-insulating state of the undoped liquid encapsulated Czochralski (LEC)-grown InP can be achieved by annealing at 800–900 °C in vacuum or phosphorus ambient[3–7] is thus a very significant breakthrough in InP technology. Although a great deal of interest has been attracted by this transition from *n*-type to semi-insulating conductivity, the role of defects involved in the compensation mechanism is still poorly understood and under investigation.

As a sensitive probe for vacancylike defects, the positron-annihilation technique can be employed to obtain microscopic information of defects, such as vacancy size, concentration, charge states, and chemical surroundings of vacancylike defects.[8,9] The present knowledge of positron-annihilation defect identification in InP defects may be summarized as follows. (i) Vacancy defects are usually present at low concentration in as-grown *p*-type SI materials, and *n*-type materials giving mean lifetimes in the range 243–247 ps which are longer than the bulk lifetime (236–241 ps),[10,11] although it appears that such trapping is not present in all material.[12,13] The typical positron lifetime associated with the trapping sites is in the range 265–275 ps, suggestive of either V_{In} or V_{P} monovacancy trapping. (ii) The mean lifetimes found in *n*-type and SI materials are generally a few ps longer than those in *p*-type materials, indicating the presence of more trapping centers.[10,11] Some *n*-type trapping centers can thus be associated with the phosphorus vacancy V_{P} [positron lifetime ~ 267 ps (Ref. 9)] that is expected to become neutral or negatively charged with the Fermi energy in either the middle or the top of the band gap.[14,15] The indium vacancy V_{In} [positron lifetime ~ 283 ps (Ref. 9)] appears to be the dominant trapping center irrespective of conductivity type. (iii) Electron-irradiation studies have revealed that although Frenkel pair defects produced in both sublattices have annealed out by ~ 250 K, fractions of V_{In} and V_{P} produced under irradiation are not annealed out at room temperature, and that these are stable to higher temperatures.[10,12,16,17] This concurs with the observation that both V_{In} and V_{P} (or related complexes) are stable, and are found in as-grown material.

In this work, positron-annihilation lifetime spectroscopy has been employed, probably for the first time, to study defect configurations in *n*-type undoped LEC-grown InP that has been made semi-insulating through long-time annealing at 950 °C. As with other observers,[10,11] we find in the as-grown state a degree of positron trapping into what are probably either V_{In} or hydrogen-V_{In} complexes. The infrared measurements reveal the presence of the shallow donor complex $V_{\mathrm{In}}\mathrm{H}_4$ that is dominant in making the as-grown material *n* type.[18,19] The annealed material reveals both a significant increase in the mean positron lifetime, indicating increased vacancy trapping, and a total absence of the $V_{\mathrm{In}}\mathrm{H}_4$ complex.

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These results are found to be in good agreement with the recently proposed mechanism of P_{In} antisite formation, which shows that the $V_{In}H_4$ complex dissociates into $V_{In}H_n^{(3-n)-}(0 \leq n \leq 3)$ deep acceptorlike defects upon annealing. The midgap P_{In} antisite deep donor forms through the recombination of a V_{In}^{3-} with a neighboring P atom to such a degree that the remaining annealed-in deep acceptors are compensated resulting in the semi-insulating form.[19] The positron lifetime results also indicate a longer 330-ps component that could possibly be associated with the $V_{In}V_P$ divacancies, and the removal of P atoms from their correct lattice sites.

II. EXPERIMENT

The sample used in this work was *n*-type ($n = 3.4 \times 10^{15}$ cm^{-3}) undoped LEC-grown InP, grown by the phosphorus *in situ* injection method.[20] A Bio-Rad Hall system was used to measure the resistivity and carrier mobility which were found to be 0.5 Ω cm and 3740 cm^2 V^{-1} s^{-1}, respectively. The sample was annealed by placing it into a quartz tube along with a quantity of red phosphorus. The samples were then annealed at 950 °C for 95 h at which the phosphorus ambient was at a pressure of 60 mbar and then cooled down to room temperature at the rate of 35 K s^{-1}. Infrared Fourier transmission measurements were carried out before and after annealing under vacuum using a NIC-170 spectrometer, with the sample at 20 K.[19]

Positron-lifetime measurements were carried out using a fast-fast lifetime spectrometer with a resolution (full width at half maximum) of 235 ps. A 3-μCi ^{22}NaCl positron source was directly deposited onto the surface of the sample in order to avoid source annihilations and the need for any correction. The samples were mounted on the copper cold finger of a closed-cycle He refrigerator cryostat for low temperature measurements. Each lifetime spectrum contained 2×10^6 counts and was analyzed using the program of POSITRONFIT.[21]

III. RESULTS AND DISCUSSION

A. As-grown material

In a defect-free crystal, positrons are delocalized and annihilate, with a single lifetime component. When there are defect-trapping centers present, where the electron density is lower, positrons will be trapped into localized states with decreased annihilation rates. The average lifetime therefore increases, and the lifetime spectrum can in general be decomposed into several exponential components. The average lifetime, being the mass center of the spectrum,

$$\tau_{av} = \sum_i N_i t_i / \sum_i N_i , \qquad (1)$$

can be obtained directly from a measured spectrum. N_i is the number of events at the *i*th time interval t_i from some suitable post-time-zero channel. This makes τ_{av} a quantity of high statistical accuracy and one independent of the decomposition process.[8] Figure 1(a) shows an average lifetime of 245 ps that varies little over the entire temperature range.

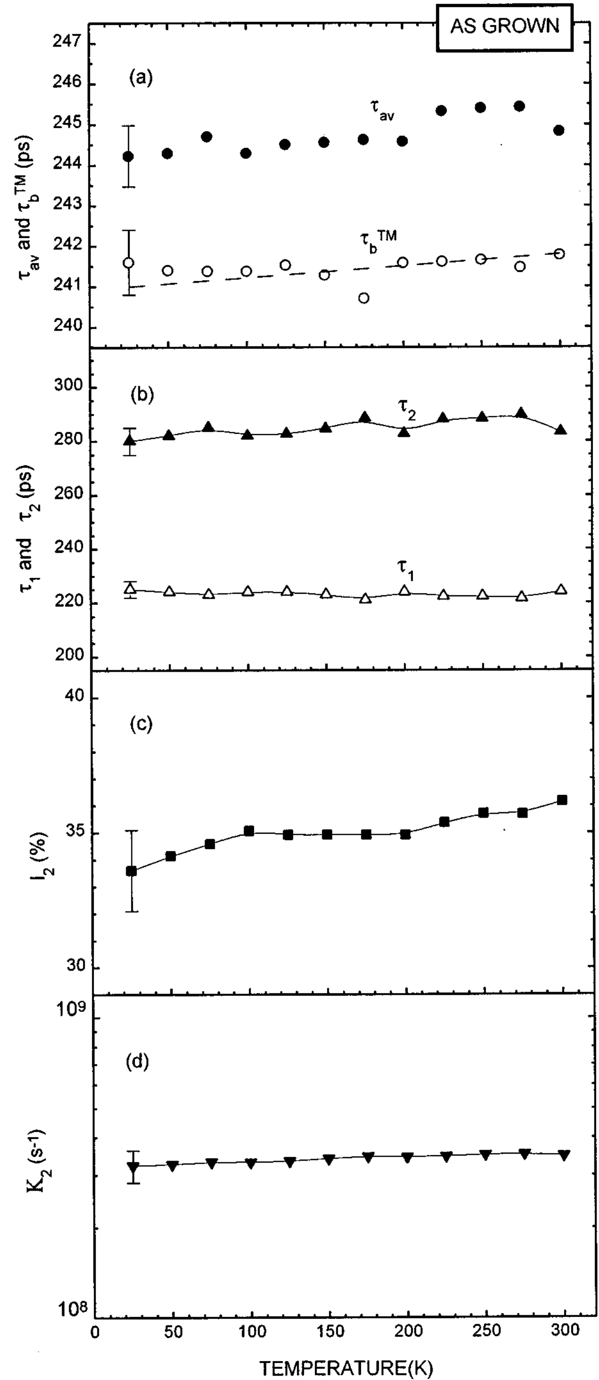


FIG. 1. Positron-lifetime results as a function of measurement temperature for the as-grown state of *n*-type LEC InP. (a) The ideal (no-trapping) positron bulk lifetime τ_b^{TM} calculated from the two-state trapping model, and the positron average lifetime τ_{av}. (b) Defect lifetime τ_2 and bulk state lifetime τ_1 as obtained from two exponential component fit. (c) Relative intensity of the defect component I_2. (d) The defect trapping rate based on the two-state trapping model.

It was found that before the sample was annealed the lifetime spectra, measured in the temperature range of 25–300 K, could be fitted well by a sum of two exponential components. The mean lifetimes τ_1 and τ_2 thus obtained are shown in Fig. 1(b), together with the intensity of the longer component I_2 in Fig. 1(c). It is reasonable to assume the

simple two-state trapping model (TM) in which positrons are transferred at some rate κ from the bulk state to the defect state.[8] According to this model the bulk lifetime of positron in a nondefected crystal is given by:

$$\tau_b^{\mathrm{TM}}=(I_1/\tau_1+I_2/\tau_2)^{-1}, \quad (2)$$

which is also shown in Fig. 1(a). The value of τ_b^{TM} is seen to be $\sim$241 ps across the entire temperature range, with a slight shortening at lower temperatures consistent with lattice contraction. The important point is that the average lifetime is 3–4 ps longer than the delocalized bulk state lifetime as a result of positron trapping by defects. The value of 241 ± 1 ps for τ_b^{TM} is in reasonable agreement with the theoretical value 240 ps,[9] and estimates from other studies on as-grown material that suggest a value in the range 234–241 ps.[10–12,16]

As seen from Fig. 1(b), spectral decomposition reveals a positron lifetime of 282 ± 5 ps, with an intensity of around 35%. Defect lifetimes around this value have often been reported in electron-irradiated material, and have been associated with the indium vacancy V_{In}. For example, Törnqvist *et al.* attributed a 283 ± 7-ps component to V_{In},[17] while Bretagnon, Dannefaer, and Kerr attributed second lifetime components in the range 263–272 ps to V_{In} (Ref. 10) and V_{In} interstitial complexes.[16] Chen, Hu, and Wang, finding a similar $\sim$270-ps component in as-grown InP of all conductivity types, concluded that the defect center must be dominantly due to V_{In} since V_{P} would be positively charged and repulsive to positrons in *p*-type material.[11] The V_{In} assignment is also supported by theoretical calculations that place the lifetime of positrons trapped in V_{In} at 280–290 ps.[19,22] The evidence is thus compelling that the trapping site we observe in the as-grown state is, even if not the isolated V_{In} some complex involving V_{In}.

To estimate the concentration of the V_{In}-related trapping site, we first compute the trapping rate. This may be done using the formula

$$\kappa(T)=\frac{\tau_{\mathrm{av}}-\tau_b^{\mathrm{TM}}}{\tau_2-\tau_{\mathrm{av}}}\frac{1}{\tau_b^{\mathrm{TM}}}, \quad (3)$$

which is derived from the simple two-state trapping model.[8] The variation of κ with T is shown in Fig. 1(d), and is seen to change little over the entire temperature range. The concentration of positron trapping defects C can be obtained by

$$\kappa=(\mu_v/N_{\mathrm{at}})C, \quad (4)$$

where κ is the defect trapping rate, μ_v is the specific positron trapping rate, and N_{at} is the number of sublattice atoms in unit volume.[23] Taking μ_v to be 4.5×10^{14} s^{-1} for neutral vacancies,[24] and N_{at} to be 1.98×10^{22} cm^{-3} for InP, the concentration of positron vacancy traps is found to be $\sim 1.5\times 10^{16}$ cm^{-3}.

A complication with assigning the observed 282-ps component to V_{In} is that the expected charge state of this defect, as judged from theoretical ionization levels,[15] is $(3-)$, and as such a strong increase in the positron trapping related parameter I_2 should be expected at low temperature.[23] Since our experimental results reveal no such variation of I_2, and indeed a slight decrease at low temperature is noted, the suggestion of V_{In}^{3-} trapping is questionable. However, a number of observations can be made. The first is that impurity shallow acceptors (mainly Zn, Mg, Ag, and Ca) are known to be present in the InP material[19] at the 2×10^{16}-cm^{-3} level. These, being $(1-)$ in their ionized states, are expected to form shallow positron traps and thus compete with vacancy trapping as the sample temperature is lowered, thus removing the expected temperature dependence. Second, the V_{In} defect may not be in its simple isolated form, but is likely to be complexed with hydrogen which is abundant in as-grown material. The presence of hydrogen atom(s) in association with V_{In} may only cause a small difference from the lifetime value. One form of V_{In} complex, $V_{\mathrm{In}}H_3$, is neutrally charged,[18] and could be the sought for trapping site. The other species $V_{\mathrm{In}}H_2$ and $V_{\mathrm{In}}H$ are expected to be singly and doubly negatively charged, respectively, and their presence would imply the need to invoke shallow trapping once again to explain the observed I_2 temperature dependence.

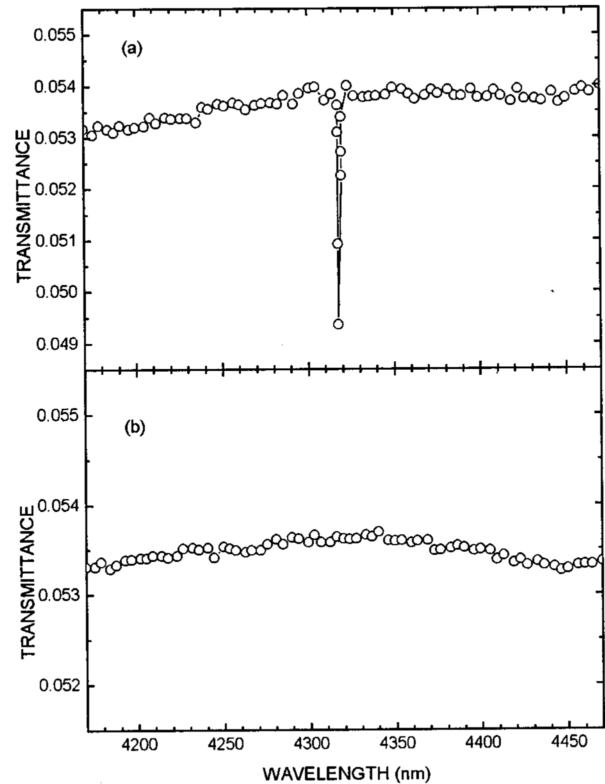


FIG. 2. FT-IR transmission spectra taken (a) before annealing and (b) after annealing. The absorption peak seen in (a) at the wavelength 4320 nm is the local vibration mode of $V_{\mathrm{In}}H_4$ complex.

The presence of hydrogen in the as-grown InP in the form of the $V_{\mathrm{In}}H_4$ complex is shown clearly in Fig. 2(a) through its Fourier transform (FT)-IR absorption peak at wavelength 4320 nm. From the estimated absorption coefficient of this line, the intensity of this peak gives a $V_{\mathrm{In}}H_4$ concentration of at least $\sim 10^{16}$ cm^{-3}. It is tempting to consider this complex as the positron trapping center, especially because its concentration is so close to that estimated from the positron trapping rate. However, there is a major objection to such an assignment. In the first place it is known that $V_{\mathrm{In}}H_4$ is dominantly ionized at room temperature, and is a major contribu-

tor to the materials' n-type conductivity.[19] It is thus in the positively charged state $(V_{\mathrm{In}}\mathrm{H}_4)^+$ state,[18] and as such is not expected to trap positrons. The fraction of the complex in the $(V_{\mathrm{In}}\mathrm{H}_4)^0$ state is estimated to be less than 10%, and is too small to explain the observed concentration of trapping centers.

B. Annealed semi-insulating material

After the sample was annealed, the material became semi-insulating with a room-temperature resistivity of $2.8\times10^7\ \Omega\,\mathrm{cm}$. At the same time, as shown in Fig. 2(b), the FT-IR measurements gave no evidence of any $V_{\mathrm{In}}\mathrm{H}_4$ absorption peak, indicating a thermal dissociation of this complex had taken place.[19] These changes can be explained by a general compensation mechanism model, which assumes that an annihilation of intrinsic defects occurs upon annealing, and that the trap levels created play important roles in the compensation.[25] The more specific model of compensation will be discussed below.

The results of the positron-annihilation lifetime measurements, in the temperature range of 25–300 K after annealing, are shown in Fig. 3. As seen from Fig. 3(a), the average positron lifetime τ_{av} has increased from the as-grown value of 245 ps to 250 ps, indicating a general increase in the degree of positron defect trapping. It was also found that two exponential components could no longer fit the spectra properly, and spectral decomposition into three components revealed a third component of lifetime $\tau_3\cong330$ ps, with an intensity of $\sim5\%$. The second component remained with a very similar lifetime $\tau_2\cong285$ ps. The 330-ps component is indicative of a defect with a larger open volume, and suggests a divacancy trapping center. Indeed it has been reported that the divacancy $(V_{\mathrm{In}}V_{\mathrm{P}})$ and divacancy-interstitial complexes in InP have positron lifetimes of 338 and 340 ps, respectively.[16,22] The presence of the 285-ps component suggests that some V_{In}-related defects remain after annealing.

Solution of the positron annihilation rate equations in a three-state trapping model, assuming two different trapping rates κ_2 and κ_3 into the two different sites, yields the set of equations[8]

$$\tau_b^{\mathrm{TM}}=(I_1/\tau_1+I_2/\tau_2+I_3/\tau_3)^{-1},$$

$$\kappa_2=(1/\tau_1-1/\tau_2)I_2, \tag{5}$$

$$\kappa_3=(1/\tau_1-1/\tau_3)I_3,$$

where I_2 and I_3 are the relative intensities of the two defect components. Figure 3(a) shows that the bulk lifetime τ_b^{TM} is still around 241 ps. Since the value derived from the three-state trapping model is in good agreement with the preanneal value of τ_b^{TM}, the reasonableness of the three-state model in describing the system after annealing is indicated. The fitting results for both as-grown and annealed cases are listed in Table I. The values of κ_2 and κ_3, calculated in this model, are shown in Fig. 3(d). These values allow us to estimate the concentration of the V_{In}-related defect (285 ps), and of the divacancy (330 ps) in the semi-insulating form. Using the same specific trapping rate as used for the as-grown case, the values obtained are 1.6×10^{16} and $3.0\times10^{15}\ \mathrm{cm}^{-3}$, respectively.

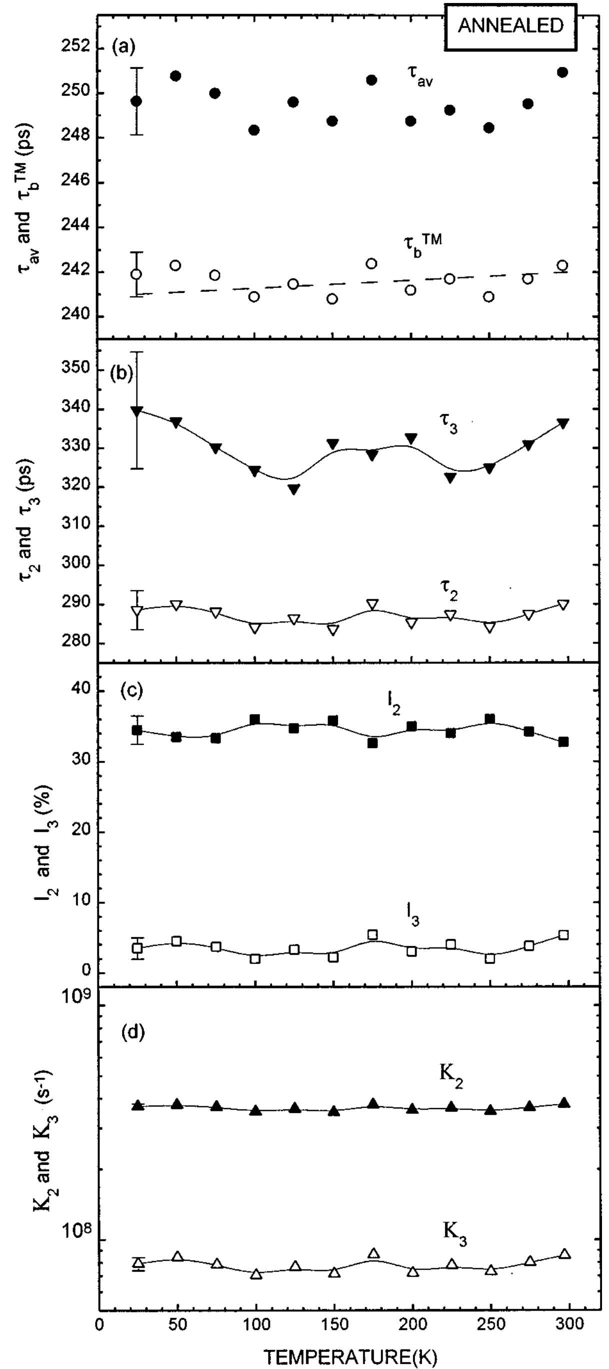
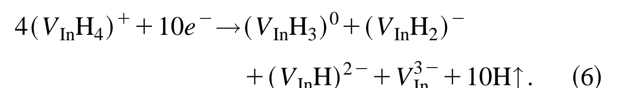


FIG. 3. Positron-lifetime results as a function of measurement temperature for the annealed SI-InP. (a) The ideal (no-trapping) positron bulk lifetime τ_b^{TM}, calculated from the three-state trapping model, and the positron average lifetime τ_{av}. (b) Defect lifetimes τ_2 and τ_3 as obtained from the three-exponential-component fit. (c) Relative intensities I_2 and I_3 of the two observed defect components. (d) The trapping rates κ_2 and κ_3 of the two defects based on the three-state trapping model.

Following the model of Ref. 19 the disappearance of the $V_{\mathrm{In}}\mathrm{H}_4$ FT-IR absorption peak arises from the dissociation of the $V_{\mathrm{In}}\mathrm{H}_4$ complexes into $V_{\mathrm{In}}\mathrm{H}_n^{(3-n)-}(0\leqslant n\leqslant2)$ complexes, and finally the isolated V_{In}^{3-} during annealing:

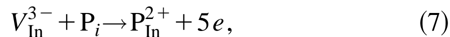


$$4(V_{\mathrm{In}}\mathrm{H}_4)^+ + 10e^- \rightarrow (V_{\mathrm{In}}\mathrm{H}_3)^0 + (V_{\mathrm{In}}\mathrm{H}_2)^- + (V_{\mathrm{In}}\mathrm{H})^{2-} + V_{\mathrm{In}}^{3-} + 10\mathrm{H}\uparrow . \tag{6}$$

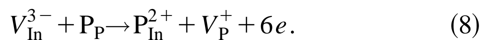
TABLE I. Positron annihilation lifetime results before and after annealing.

	Before annealing	After annealing (950 °C)
I_2 (%)	35	33
I_3 (%)	/	5
τ_1 (ps)	223	218
τ_2 (ps)	282	285
τ_3 (ps)	/	335
κ_2 (s^{-1})	3.3×10^8	3.6×10^8
κ_3 (s^{-1})	/	7.5×10^7
τ_b^{TM} (ps)	241	241
τ_{av} (ps)	245	250

The V_{In}^{3-} then either captures an interstitial P_i atom or a neighboring P_P atom to form the EL2-like antisite defect (P_{In})



$$V_{In}^{3-}+P_i\rightarrow P_{In}^{2+}+5e, \tag{7}$$



$$V_{In}^{3-}+P_P\rightarrow P_{In}^{2+}+V_P^{+}+6e. \tag{8}$$

The compensation of hydrogen associated V_{In} deep acceptor levels and other residual acceptor impurities by the EL2-like P_{In} antisite deep donor produces the semi-insulating state.

The above model allows a relatively easy interpretation of the positron lifetime data. The $V_{In}H_n^{(3-n)-}$ products of the above dissociation, being V_{In} related, are anticipated to be additional positron traps with lifetimes of around 280–290 ps. However, the trapping rate into this monovacancy component has not increased significantly, which would suggest that the hydrogen evolution pathway expressed in reaction (6) is a secular equilibrium, with the concentration of intermediate species $V_{In}H_n^{(3-n)-}$ remaining approximately constant. With regard to the 330-ps lifetime component, reaction (8) gives a possible source of a divacancy defect. V_P formed through this reaction could be in the vicinity of an indium vacancy and form the $V_{In}V_P$ divacancy or hydrogen associated forms of this defect. Clearly more studies at intermediate annealing times could give further evidence to support this picture.

IV. CONCLUSION

Positron-lifetime measurements carried out on LEC-grown InP have shown that the average positron lifetime increases from 245 to 250 ps upon annealing, manifesting stronger positron trapping effects in the annealed state. Two defect components are separated in the annealed semi-insulating state. The first is of similar structure to the trapping center found in the as-grown InP, and has a lifetime ~285 ps. It is argued that this is most likely to be due to hydrogen V_{In} complexes of the form $V_{In}H_n^{(3-n)-}(0\leq n\leq3)$, since the lifetime value is close to the positron lifetimes of indium-vacancy-related defects seen by others. A second defect lifetime component of ~330 ps, found in semi-insulating form, is most likely to be due to the $V_{In}V_P$ divacancy or possibly related complexes. Both these defects are suggested to originate from the thermal dissociation of the $V_{In}H_4$ complex.[19] Positron trapping rates into both defect types are found to be essentially independent of temperature over the wide temperature range of 25–300 K, indicating either that these defects are neutrally charged, or that competing shallow traps exist having a trapping rate which follows that of the vacancy defects.

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