On the Photo-Ionized DX Centers in Te-Doped $Al_{0.46}Ga_{0.54}As$

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Abstract

Overview of the investigation of DX centers in $Al_xGa_{1-x}As$ has been briefed. Our recent works on optical absorption and its magnetic circular dichroism (MCDA) of photo-ionized DX centers in Te-doped $Al_xGa_{1-x}As$ (say Te:DX^0 center) have been measured when $x=0.46$. Optical detection of electron paramagnetic resonance (EPR) of the Te:DX^0 center has been observed through the change of MCDA at the resonant condition. It gives $g=1.62\pm0.02$ and half-width (FWHM)$=14\pm2$ mT. No hyperfine (*hfi*) splitting is detected. Future problem for the study of Te:DX^0 center is proposed.

§1. Introduction — Historical Overview

The DX centers in $Al_xGa_{1-x}As$ are deep donors introduced by doping with group Ⅳ (Si and Sn) or Ⅵ element of Te when x exceeds about 0.22. Here, D stands for a shallow donor and x presents an unknown defect associated with D[1]. The early studies of DX centers were carried out mostly through the measurements of optical processes (luminescence and Raman scattering *etc.*), electrical transport processes (conductivity, Hall effects, and DLTS *etc.*) by Lang and Logan in 1977[2], Lang in 1985[3], Mooney *et al.* in 1987[4], Mooney in 1990[5], and Bourgoin in 1990[6]. From these results, it has been clarified that DX centers have a much larger photo-ionization threshold energy (more than 1 eV) than the thermal ionization energy (0.2 eV for Si). In addition to these properties, DX centers have unusual properties such as leading to a persistent photoconductivity (PPC) when they were photo-ionized at low temperatures[1]. The PPC leads to the persistent refractivity change: The effect would be deduced to an optical nonlinearity[7,8]. This may provide a profound possibility for application as holography and memory storage.

Important properties of DX centers and its models proposed previously are still controversial. The recent argument is particularly focused on their microscopic configuration including the charge states of the ground and its relaxed state of the DX centers after photo-excitation. This depends on to check whether a large lattice relaxation (LLR) associated with it does exist or not. Details of these results are

summarized in Refs. 9-12.

A substitutional donor in its neutral charge state is expected to have a paramagnetic ground state (GS). However, when the specimens were cooled in the dark, no EPR was found by Mooney *et al.* in 1989[13] and von Bardeleben *et al.* in 1989[14]. This fact implies that the DX center has a diamagnetic GS. We call it the DX^- center. As shown in Refs. 13 and 14 and by von Bardeleben *et al.* in 1990[15], EPR was observed only after photo-excitation with light of energy exceeding the photo-ionization threshold.

In 1989, Chadi and Chang proposed that donor is not stable in the neutral paramagnetic charge state D^0 but captures a second electron to form the DX^- center[16]. It shows negatively charged GS, in which the dopant atom goes to an <110> off-center position causing a sort of the LLR after trapping an extra electron. In other words, the whole two-electron system in the DX^- center possesses a negative-U character in which the energy is lowered by the LLR. The same model was proposed independently by Morgan[17]. Toyozawa proposed that this sort of structure bistability is caused by short-range interaction potential[18].

After photo-ionization, the DX^- center is turned into a neutral paramagnetic charge state, DX^0 center, which can be detected by using paramagnetic resonance technique (EPR). The neutral DX^0 state must be thermodynamically unstable (metastable), but obviously should play a role in its carrier capture and emission processes as an intermediate state ($DX^- \leftrightarrow DX^0+e \leftrightarrow DX^++2e$), where superscripts show only charge state, independent of their microstructures[19]. Here, we have still ambiguous problem left whether the DX^0 is coincident with a shallow donor itself or a dopant with a small amount of LR.

A new method of optical detection of EPR has been developed in Spaeth's laboratory at Paderborn in Germany[20]. This is a MCDA-tugged EPR. The MCDA is the differential absorption of left and right circularly polarized light which propagates in the direction of an external magnetic field (Faraday configuration). The MCDA signal intensity is proportional to the spin polarization (P_S) in the Zeeman split levels of a paramagnetic defect having an orbital singlet ground state of A_1 symmetry[20,21]. Hereupon we discuss solely on the paramagnetic component of the MCDA. By sending microwave to cause resonant transition between the Zeeman split levels, the P_S is reduced to zero. So that the MCDA is diminished to give rise to the EPR lines. This is a working principle of the optical detection of EPR (ODEPR). As the MCDA of the paramagnetic centers depends on temperatures and magnetic field, one may easily distinguish the para- and dia-magnetic GS.

The EPR for DX centers doped with group Ⅳ donor (say Ⅳ:DX) have been well investigated. In Refs. 13 and 14, the single-line Sn and Si EPR spectra were first observed and interpreted as due to *a shallow excited hydrogenic state associated with the DX centers* (*EMT*). However, Fockele *et al.*[22,23] showed that this must be revised. Neither MCD nor ODEPR spectra are those of an EMT associated with a conduction band minimum. Because an optical transition from EMT donors to the conduction bands would not be high of about 0.73 eV. For a hole transition to the valence band

much larger photon energy is required[24]. Futhermore, the Sn hyperfine interaction (*hfi*) of 10.1 GHz observed by von Bardeleben *et al.*[25] and Ref. 22 corresponds to the spin density of about 13% relative to an Sn 5s orbital. The spin density of a full, unpaired 5s electron was calculated to be 73.9 GHz (^{119}Sn) making use of the local spin density approximation[26-29]. Thus, 13% localization is typical for a deep defect. Meyer *et al.* similarly estimated that the localization of 15% for the unpaired electron at the ^{75}As central nucleus in the EL2 defect[30]. As a conclusion, Sn is found to form a deep paramagnetic state Sn:DX^0 with A_1 symmetry, while Si:DX^0, a shallow EMT, is related to the X-band minimum. A contemporary review of the ODEPR of DX centers was published by Spaeth and Linde in 1994[31].

However, as for VI group donor element like Te, no convincing ODESR signals have been obtained before issued our work[32]. In Ref. 15, an anisotropic EPR line was observed for $x>0.3$ after photo-ionization and was assigned as Te^0. Even though, it was not clear whether the EPR line was due to a deep A_1 state or an EMT state (*hydrogenic state*) yet. In 1993 Peale *et al.* failed in its magneto-optical detection for a substrate-free Te-doped sample with $x=0.35$[33].

The direct measurement of optical absorption for $Al_xGa_{1-x}As$ has not been tried by 1992. Insufficiently thin thickness of specimens suffers its observation. In 1992, Mori *et al.* have succeeded in its direct measurements for the specimens offered from Hitachi Cable Co. Ltd.[34]. In addition to infrared absorption bands due to Te:DX^- centers, they could observe a new band peak of 0.56 eV after photo-ionization of Te:DX^- centers. The new band is associated with a metastable Te^0 donor or Te:DX^0[34]. A year later, Kaczor *et al.* confirmed this result by the other method[35]. They also observed IR absorption at lower energy range that is associated with the shallow EMT state of donor atoms. Based on these works, the ESR of MCDA of DX^0 centers has been successfully carried out in the University of Paderborn[32]. The result will be introduced in § 2.2.

§2. Experimental

(2.1) Optical absorption

The optical absorption spectrum of a defect center is one of the most important measures to investigate its microscopic structure. However, its direct measurement has been prohibited because of thin thickness of specimens (~ a few μm) of AlGaAs specimens. Their data have been obtained indirectly from spectral dependence of photoconductivity or MCDA measurement so far. Thanks to Hitachi Cable Co. Ltd., they kindly supplied us thick specimens of n-$Al_xGa_{1-x}As$ with several 200-300 μm grown by liquid-phase epitaxy. Here, the concentration of Te was $5\sim10\times10^{17}$ /cm^3 and x varies up to 0.46. The thickness of specimens is suitably enough for direct measurement of absorption spectrum.

Optical density for Te:DX centers in $Al_xGa_{1-x}As$ with $x=0.46$ is observed at fixed temperature over the range from 77K to room temperatures[34]. A series of experimental data are plotted in Fig. 1 as a function of photon energy E_{ph}. Solid curve (a) is the

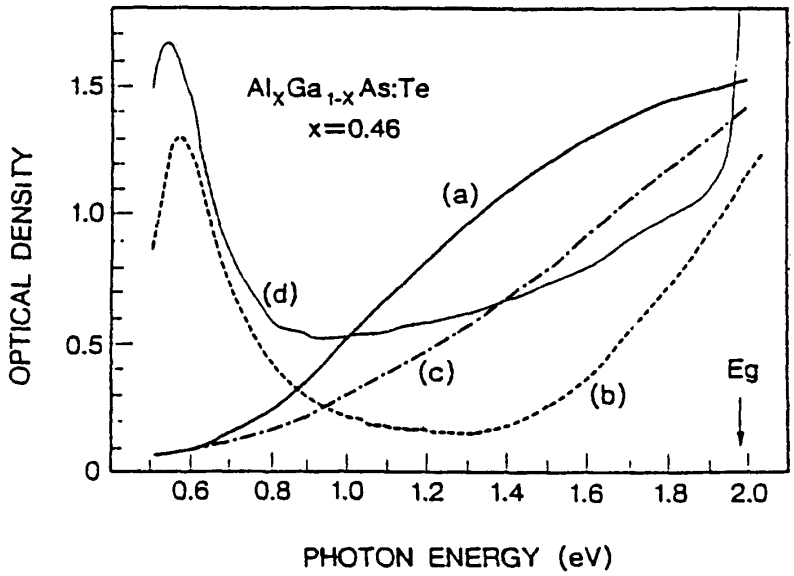

Fig. 1 Optical absorption spectra of 300 μm thick Te-doped $Al_xGa_{1-x}As$ with x=0.46 are shown. Curves (a) is taken at thermal equilibrim at 77K (solid lines). (b) non-equilibrium under 1.17 eV YAG laser excitation at 77K (doped lines). (c) after termination of YAG laser at 77K (chained lines). (d) thermal equilibrium at 300K (thin solid lines). Data are taken from Ref. 34.

OD spectrum measured at 77K by relatively weak light after cooling specimen down to 77K in darkness. We have checked that curve (a) is nearly coincident with the cross section spectrum of photo-ionization reported previously[9]. Thus, we may assume that the wide absorption peaked at 1.5 eV is related to the optical absorption due to the Te: DX^- center. Curve (b) is obtained during simultaneous irradiation of intense light of 1. 17 eV from a Nd^{3+}: YAG laser that proceeds photo-ionization of the Te:DX^- center to form the Te:DX^0 center. Here, the increase of the infrared absorption band peaked at 0.56 eV is observed at the expense of the Te:DX^- center peaked at 1.5 eV. We may ascertain that the new peak corresponds to the absorption due to the Te:DX^0 center. To our best knowledge, this is the first direct observation of the Te:DX^0 center band. The 0.56 eV band is thermally unstable at 77K. After termination of the YAG laser light, the absorption spectrum is varied as plotted in curve (c). It shows that the 0.56 eV band completely disappeared, but the 1.4 eV is recovered partially. This reveals that, except for 0.56 eV band, another metastable and optically insensitive unknown state could be formed by intense irradiation of the Te:DX^- center.

The absorption observed after increasing the specimen temperature to 300K is plotted in (d). Again the 0.56 eV band appears seemingly at the expense of the DX^- center band under thermal equilibrium conditions. This is quite difficult phonomena to understand. Because this may occur in the case when the thermal depth of the Te:DX^0 center would be less than that of the Te:DX^- center. The energy level relation between optical and thermal depth is inverted from that at low temperatures. Hereupon, a question arises whether this 0.56 eV at thermal equilibrium would be paramagnetic or not. We may suggest to apply the MCDA and ODEPR method to re-examine the microstructure of these DX centers formed in the thermal equilibrium.

(2.2) MCDA and ODEPR

The MCDA for the same specimen as was tested in the preceding subsection is measured at 3T and 1.5K in the Spaeth's laboratory. A cooled InSb detector was used in the spectral range of 0.5 eV to 1.0 eV and a cooled Ge detector between 0.78 and 1.53 eV. Photoconductivity was measured simultaneously.

An MCDA spectrum, that was observed after illuminating the sample (x=0.46) held

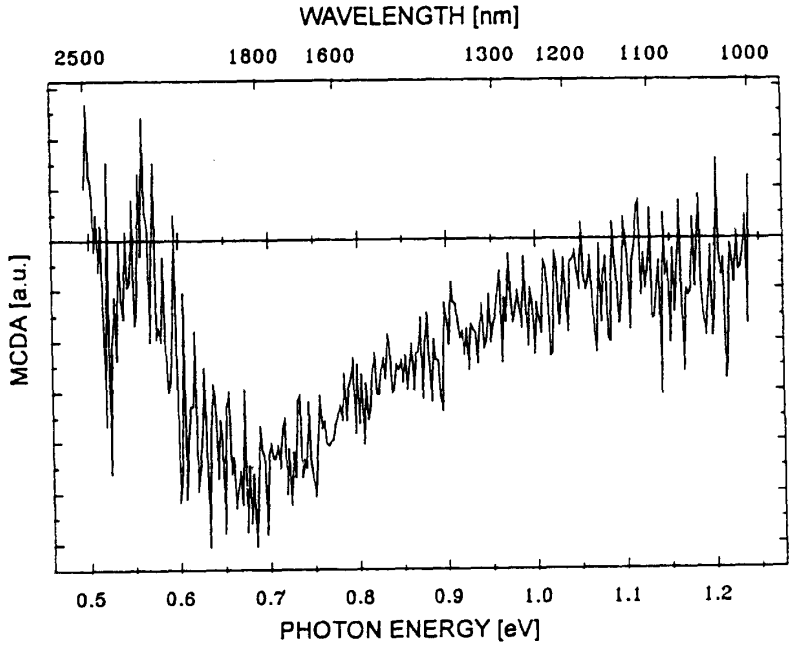

Fig. 2 MCDA of the same specimen as Fig. 1 measured at T=1.5K and B=3T after photo-ionizing the DX centers. Substrate was removed. Data are from Ref. 32.

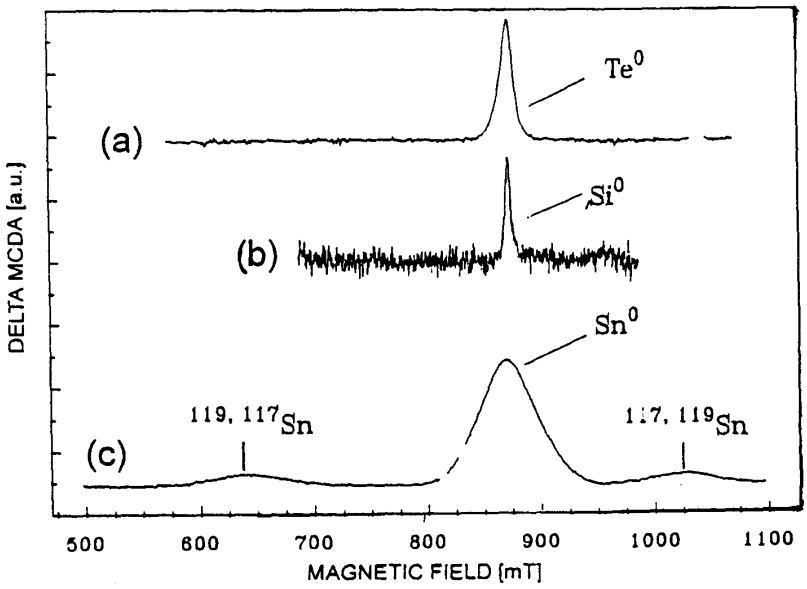

Fig. 3 ODEPR spectra of DX^0 centers in $Al_xGa_{1-x}As$: (a) Te-doped measured at 0.8 eV and B=1.5T for x=0.46. Taken from Ref. 32. (b) Si-doped measured at 0.8 eV and B=1.5T for x=0.5. Taken from Ref. 31. (c) Sn-doped measured at 1 eV for x=0.35. Taken from Ref. 23 and 31. All the spectra were presented for a microwave frequency of 24 GHz.

at 1.5K with a very faint (>1mW) measurement light of photon energy exceeding 0.6 eV, is plotted in Fig. 2 as a function of E_{ph}. This spectrum may be a one-half part for high E_{ph} region as was expected from a whole differential shape of Fig. 1. The observation of lower E_{ph} component of the MCDA would be impossible because of lack of a suitable detector. In the limit of "zero measurement light intensity", no MCDA could be measured. This is a nice proof to show that the sample is diamagnetic after cooled in dark. It also shows that no EMT state of dopant exists. The MCDA signal reaches a saturation value depending on the E_{ph} of exciting light. It is confirmed that the E_{ph}-dependence of the saturation values of the MCDA measured at 0.77 eV shows the threshold at 0.6 eV. There is a very good agreement with the E_{ph}-dependence of the absorption cross section measured by Lang *et al.*[9]. The temperature dependence of the MCDA is also measured. It is decreased with increase of temperatures. This again shows that the optical absorption peaked at 0.56 eV in Fig. 1 originates from the P_s in a paramagnetic GS.

The ODPER spectrum for $x=0.46$ measured in the MCDA at 0.8 eV is plotted in Fig. 3 as a function of magnetic field, B. The PER line is isotropic with $g=1.62\pm0.02$ and $\Delta B_{1/2}$ (FWHM)$=14\pm2$ mT. No *hfi* splitting due to the magnetic isotope ^{125}Te (7% abundance) with $I=1/2$ could be observed. We will discuss the deficit of the *hfi* line later. In Fig. 3, ODEPR lines for Sn:DX and Si:DX are plotted as a reference[31].

After cooling the specimens in the dark, no photoconductivity could be observed at low temperatures. If the sample is irradiated with $E_{ph}=\hbar\omega>0.6$ eV a photoconductivity was measured which remains persistent after the light is switched off. The level of photoconductivity at 1.5K is very low. A phenomenon is the same as was previously observed when performing similar experiments on Sn- and Si-doped $Al_xGa_{1-x}As$ samples in the indirect gap x range[26,31] and also observed by Mizuta *et al.* in 1988[36].

In order to establish a correlation between the PPC and the MCDA a following series of experiments were carried out in Ref. 32. The samples was first cooled in the dark to 1.5K and then illuminated with 0.8 eV light for a certain time. The MCDA at 0.8 eV was measured at 1.5K. Thereupon the sample is heated to 40K, at which temperature the PPC can be measured. At temperature below 40K the PPC decreases and is not measurable at 1.5K because of freeze-out of electrons in *the unknown shallow states*. The sample was then heated to 200K and cooled to 1.5K to make sure that the initial state was obtained again. Now the same illumination and heating cycle was performed for another duration of the illumination.

§3. Discussion

We summarize recent experimental results done for the Te:DX centers. The work was at first done by Mori *et al.* at Osaka City University[34] and Linde *et al.* at University of Paderborn[35] with using the same specimen of Te-doped $Al_xGa_{1-x}As$ prepared by Hitachi Cable Co. Ltd. The author is involved as one of co-authors in both successive works.

The appearance of the MCDA and of the ODPER are associated with a photoionization process and optical absorption of the sample. The photo-ionization threshold agrees with that known for Te:DX centers[9]. Thus, a metastable and paramagnetic Te^0 state ($Te:DX^0$) is formed upon photo-ionization of the $Te:DX^-$ centers, which gives an isotropic EPR line with 15 mT width and is accompanied by photo-electrons in the coduction band (PPC). The results are analogous to those found with similar experimental techniques for Sn: and $Si:DX^-$ centers of typical Ⅳ elements.

The EPR line observed for the $Te:DX^0$ centers is not exactly similar to that for the $Sn:DX^0$ centers but is similar to that for $Si:DX^0$ centers. One difference is following. The *hfi* split lines observed for the former case did not appear in the latter. The EPR line width (FWHM) for the former (51 mT) is comparably large with that for the latter (8 mT) and the present (15 mT). The g-values observed are isotoropic. From the large *hfi* splitting for the $Sn:DX^0$ centers (340 mT), the s-like spin density at Sn nucleus is entimated to be 13%. A theoretical value of s-like spin density for the deep A_1 donor calculated by Overhof gives good agreement[26-29]. On the other hand, the *hfi* splitting of $Te:DX^0$ centers did not appear experimentally. Overhof predicted the *hfi* splitting for the deep A_1 state of ^{125}Te would be as 84 mT. This could have been observed in the experiment, judging from the signal-to-noise ratio of about 50:1. From this fact, we may assume that the *hfi* constant would be possibly much less than the expected value. So that it might be included in the EPR width. Lack of the *hfi* splitting implies that the wavefunction of $Te:DX^0$ centers would not be calculated in the same way as that for the $Sn:DX^0$ centers. One of the way to resolve this discrepancy, ODENDOR measuremet should be prepared.

The disappearance of the *hfi* splitting in EPR lines described above might be caused from the quite different microscopic property of Si: and $Te:DX^0$ centers from the Sn: DX^0 centers. Besides, comparison of the shape and energy position in the MCDA band for Te (Fig. 2) with that for Si[31,32] shows the same behaviors on the optical transition. Therefore it can be explained by a Locovsky-type that is a photo-ionization transition into a conduction band[37]. The absorption cannot be due to an optical transition to either the valence band[24] or the nearest conduction band from energetical reasons. In Ref. 32, it is suggested that a transition occurs to the X_3 band minimum. The energy separation of $|X_3-X_1|$ observed is close to a theoretical value[38]. This is also in agreement with Kaczor *et al.*[35] and the previous result for Si. A very similar MCDA has been observed by the Spaeth's laboratory for shallow Te^0 and S^0 donors in GaP, which was interpreted as a transition to the L-band minimum[39].

However, there is still ambiguous point left on the microstructure of the 0.56 eV absorption band. In Ref. 19 Dobaczewski and Kaczor analyzed their photo-ionization process of the $Te:DX^-$ center, and postulated that the intermediate (*metastable*) state corresponding to the DX^0 center is not the effective mass X- or -like excited state of the DX center, but a *neutral, most likely resonant, state strongly coupled to the lattice, similar to the ground* DX^-. A year later, Kaczor *et al.* attributed it to a transition from *a shallow X-like donor* to a higher X minimum (of the X_3 symmetry) of tthe

conduction band[35]. Consequently, they determined X_3-X_1 energy splitting that is close to the theoretical value in Ref. 38. However, it is hard to recognize that both models are quite the same.

According to our observation shown in Fig. 1, the 0.56 eV band is from *thermally unstable (metastable) state* at 77K. So that, after termination of the photo-ionized light, it disappeared and instead the 1.5 eV band due to the Te:DX^- center is partially recovered. This is one of the reasons to believe the thermally non-equilibrium condition at 77K. On the other hand, with increase of specimen temperatures to room temperatures, it has been confirmed that the 0.56 eV band is increased at the expense of the Te:DX^- center absorption (at 1.46 eV). This occurs in thermal equilibrium condition at room temperatures. The fact is coincident with our result as shown in Fig. 1(d). However, in order to explain this fact we should assume that thermal ionization energy of the Te:DX^- center at room temperature tends to become much smaller value than that of the Te:DX^0 centers. This assumption is quite contrary from the fact at 77K (in thermal non-equilibrium condition) where thermal depth of the Te:DX^0 state would be deeper than Te:DX^0 centers. The investigation of the origin of this discrepancy is left unexplored.

For these purposes, we may suggest to check the MCDA or ODEPR for these centers in the thermal equilibrium as in the same manner done for Te:DX^0 centers that were created at 1.5K.

§4. Conclusion

The optical absorption, magnetic circular dichroism, and optical detection of DX^0 centers in Te-doped $Al_xGa_{1-x}As$ with $x=0.46$ have been observed. From the study of these quantities, microstructure of Te:DX^0 centers is partially clarified. For further extensive study, several future project to explain details of microstructure has been proposed.

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