

***DX*-center transformation of Te donors in GaSb under hydrostatic pressure**

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We have observed the transformation of Te shallow donors in GaSb into *DX* centers at hydrostatic pressures of 27.8 ± 2.6 kbar. The position of the Te *DX* energy level at zero pressure is calculated to lie 300 ± 70 meV above the conduction band at atmospheric pressure, consistent with the theory that in the III-V compounds the *DX* centers line up in energy with respect to the vacuum level within experimental error. This binding energy at zero pressure of the Te *DX* compares well with the value of 210 meV calculated from the cation-cation bonded *DX*-center model recently proposed by Park and Chadi. At pressures where the Te shallow donor into *DX*-center transformation has taken place we observe evidence of the existence of a bound phonon associated with the Te *DX* center. From its observed pressure dependence the LO optical phonon Grüneisen parameter is calculated to be $\gamma_{LO} = 0.93 \pm 0.09$. [S0163-1829(98)11419-4]

The *DX* center is a deep defect found in many *n*-type compound semiconductors and their alloys. *DX* centers were first discovered in $\text{GaAs}_{1-x}\text{P}_x$ by Craford *et al.*,¹ and have been studied extensively in Si-doped *n*-type $\text{A}_x\text{Ga}_{1-x}\text{As}$ for $x > 0.22$ by Lang and co-worker,^{2,3} who created the name of *DX* center. Certain shallow substitutional donors in III-V compound semiconductors transform into *DX* centers under hydrostatic pressure, for example, Si in GaAs (Refs. 4 and 5) and S in InP.⁶ These experiments demonstrated that *DX* centers are substitutional shallow donors⁷ that undergo a structural change resulting in the formation of a deep level under certain conditions of alloying or hydrostatic pressure.

DX centers are characterized by several unusual properties, including a large difference between their thermal and optical ionization energies and extremely small electron capture cross sections that at low temperatures give rise to persistent photoconductivity. These features of *DX* centers are interesting from the viewpoints of both physics and technological applications since the electrical characteristics of a semiconductor containing metastable defects are affected by the relative stability of the shallow and deep configurations of the defects.

In addition to the examples mentioned above, *DX* centers have also been observed to form⁷ in Te-doped $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ at Al fractions above 0.2. This result combined with the similarity between the band structures of these compounds with those of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ alloys and the suggestion that *DX* centers might be a general phenomenon in all III-V compounds⁸ prompted the question as to the existence of Te *DX* centers in GaSb. Deep level transient spectroscopy

(DLTS) measurements of sulfur-doped GaSb have shown that the S donor coexists as a shallow donor and as a *DX*-like deep level at atmospheric pressure and low temperatures.^{9,10}

In GaSb at atmospheric pressure, the L_1 conduction-band minima in the (111) direction lie only 0.08 eV above the absolute conduction-band minimum at the Brillouin-zone center (Γ_1). The X_1 minima near the (100) zone boundary lie about 0.43 eV above the Γ_1 minimum.¹¹ Upon the application of hydrostatic pressure, the Γ_1 and L_1 minima move upwards and the X_1 minimum downwards in energy with respect to the valence band. Because the Γ_1 minimum has a larger pressure coefficient than the L_1 minimum, the L_1 minima become lower in energy than the Γ_1 minimum roughly above 10 kbar. At still higher applied pressures (above about 50 kbar) the X_1 conduction-band minima fall below the L_1 conduction valleys in energy and thereafter are the absolute minima.

The pressure dependence of two group-VI elements that form donors in GaSb, Se, and Te, has been studied previously by observing the change in resistivity at pressures as high as 50 kbar.^{12,13} In those studies it was thought that the increase in resistivity above 10 kbar in GaSb:Se was due to the greater effective mass of the Se shallow donor associated with the L_1 minima.¹² However, recently it has been suggested that these observations may indicate the formation of *DX* centers.¹⁴ Although a decrease of almost one order of magnitude of the free carriers was observed for hydrostatic pressures above 38 kbar for the case of Te donors, no similar association or assignment to a localized donor was proposed,¹³ perhaps due to the moderate change in resistivity as compared to the three and five orders of magnitude change observed for Se- and S-doped samples, respectively.

In this work, we report on the observation of a freezing out of free carriers at low temperatures and hydrostatic pressures of 30 kbar and above and on the appearance of persistent photoconductivity in this material under these conditions. These findings are consistent with the existence of Te *DX* centers at these pressures.

The samples used were GaSb:Te with free-carrier concentrations of 0.5 and $1.3 \pm 0.3 \times 10^{18} \text{ cm}^{-3}$. The samples were thinned down to 50 μm in thickness and were cut into small disks 300 μm in diameter using an ultrasonic grinder as described elsewhere.¹⁵ Hydrostatic pressure was applied to the sample using a modified Merrill-Basset diamond-anvil cell with liquid nitrogen as the pressure medium. The far infrared transmission (FIRT) of the sample was measured with a Digilab FTS-80E vacuum Fourier Transform Spectrometer and a small Ge:Cu photoconductive detector mounted directly behind the pressure cell. We measured the pressure in the cell before and after the (IR) measurements, by means of the pressure dependence of the wavelength of the R_1 and R_2 fluorescence lines of the Cr^{3+} ion in ruby. The low-temperature pressure, at which the FIRT is observed, was estimated from a calibration previously obtained using the pressure dependence of the ν_3 vibrational mode of CO_2 at 4.2 K.¹⁶ It is estimated that the low-temperature pressure is around 10 kbar lower than the average of the room-temperature pressures before and after liquid-helium cooling.¹⁶ The uncertainty in the applied pressures is estimated to be ± 2 kbar. All spectra were taken at 4.5 K.

At low pressures the Te donors are all in the shallow donor state and in our samples, which were highly doped, the shallow impurity band has broadened and merged with the conduction band. Hence all of the donor electrons from Te behave like free carriers and the sample is opaque to far-infrared radiation (FIR) due to free-carrier absorption. When the sample is subjected to hydrostatic pressures of 30 ± 2 kbar or above, however, the Te shallow donors transform into their *DX* configuration. Upon cooling, the carriers become trapped at the deep *DX* levels and the sample becomes transparent to FIR. However, by shining light of energy greater than 1 eV on the sample, the *DX* centers can be converted back into their shallow configuration (persistent photoconductivity) and the sample returns to its opaque state. At low temperatures, a thermal barrier prevents these shallow donors from returning to their deep *DX* configuration. Thus, the shallow donor-to-*DX* center transition pressure is taken to be the pressure at which the sample shows this persistent photoionization.

In order to detect this persistent photoionization, the following procedure was used. First, the sample was brought to the desired pressure and cooled to liquid-helium temperatures. A reference spectrum was then taken. The light incident on the sample during this process was not of a short enough wavelength to disturb any *DX* centers that might be present in the material. Light of a much higher energy was then shined on the sample using an ordinary incandescent light bulb, converting any *DX* centers back into the normal shallow state. A second spectrum was then taken and ratioed against the reference spectrum. Any additional absorptions by the sample (for example, due to persistent photoionization of the Te *DX* centers) after the light treatment would then show up as positive peaks in the absorbance spectrum.

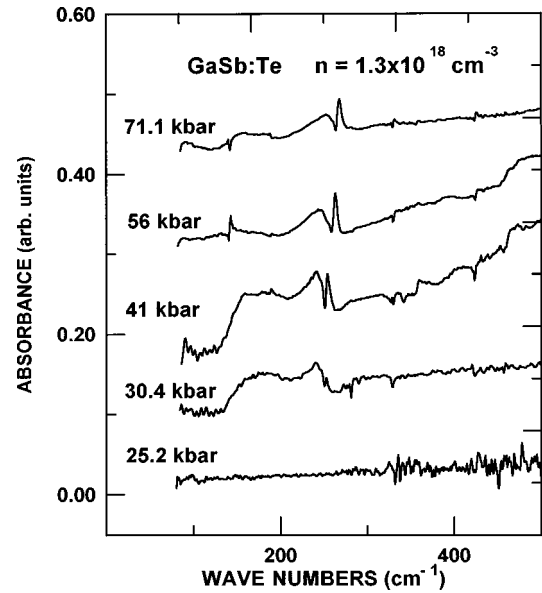


FIG. 1. Far infrared absorbance spectra by Te-doped GaSb under applied hydrostatic pressure.

In Fig. 1 absorbance spectra of the GaSb:Te at pressures of 25.2, 30.4, 56.0, and 71.1 kbar and $T=5$ K are shown. At the lowest pressure (25.2 kbar), we see that ratioing of the spectra taken before and after shining light on the sample produces a flat absorbance, indicating that there is no persistent photoionization. However, at 30.4 kbar, we can clearly see the presence of light-induced absorption. Hence, the transition pressure must be between these two pressures and is estimated to be 27.8 ± 2.6 kbar. A phonon-related sharp absorbance peak is also visible as a Fano-like resonance in the electronic continuum in the spectra recorded at 41, 56, and 71 kbar. Careful observation indicates its presence also for the spectrum taken at 30.4 kbar, as well as for all spectra recorded under applied pressures above the transition value of 27.8 ± 2.6 kbar. These peaks have a line shape similar to that of the reststrahlen band observed in reflectivity for the same GaSb sample which, at 10 cm^{-1} wide, is very narrow in this compound. On the low-energy side of this sharp peak, a broad asymmetric absorption band is seen in all spectra above the transition pressure. The spectral widths of these bands increase monotonically with increasing applied pressures from around 25 to 55 cm^{-1} for the pressure values between 30.4 and 71 kbars, respectively.

One possibility for the sharp peak is that it is a bound phonon,^{17,18} i.e., a phonon bound to either the shallow hydrogenic donor associated with the L minima or to the deep *DX* form of the Te impurity. The energy of this peak extrapolates to $238.3 \pm 1.5 \text{ cm}^{-1}$ at atmospheric pressure, which is very close to the LO phonon energy of 240 cm^{-1} at liquid-helium temperatures and atmospheric pressure.¹⁹ Bound phonons have been observed at low temperatures when the impurities are neutral and the main dipolar-active (1S-2P) transition energy of the impurity is larger than that of the LO phonon.¹⁷ Bound phonons associated with *DX* centers have been observed in GaAs under pressure after the Γ - X transition has taken place.¹⁸ However, our results as well as previous experiments have shown that Te donors associated with the L valley in GaSb have binding energies

TABLE I. Comparison of the energy positions ΔE_{DX} of Te $-DX$ centers observed in III-V semiconductors. The zero of energy is located at the Γ minimum of the GaSb conduction band.

Compound	E_g at 4.2 K (eV)	ΔE_C (meV)	E_0 (meV)	ΔE_{DX} (meV)
GaSb	0.81		0	300 ± 70
CCB model				210^a
$\text{Al}_{0.4}\text{Ga}_{0.6}\text{Sb}$	1.32 ± 0.02^b	330 ± 10^c	60^d	270 ± 30
$\text{Al}_{0.36}\text{Ga}_{0.64}\text{As}$	2.00 ± 0.05^e	$350 \pm 50^{f,g}$	100^e	250 ± 70
$\text{GaAs}_{0.64}\text{P}_{0.36}$	1.96 ± 0.05^h	$390 \pm 50^{i,g}$	70^j	320 ± 60

^aReference 33.

^bReference 28.

^cReference 27.

^dReference 1.

^eReference 2.

^fReference 29.

^gReference 31.

^hReference 32.

ⁱReference 30.

^jReference 3.

of only about 20 meV,²⁰ ruling out the possibility that any ground to bound excited state transitions of this donor could be larger in energy than the LO phonon (29.8 meV). It is also very improbable that this feature is associated with a phonon bound to the DX state since all of the DX centers are converted to the hydrogenic form of the donors by the illumination of the sample by light chosen precisely to ionize them, before taking the second spectrum to be ratioed. This experimental procedure produces the absorbance of the sample without electrons populating these centers. Hence, our experiments cannot be conclusive to the existence of phonons bound to Te DX centers in GaSb.

A second possibility is that the sharp peak is simply the LO phonon itself. Although LO excitations are normally forbidden in IR absorption, the concentration of Te impurities is high enough to affect the local translational symmetry of the crystal and hence produce q -independent impurity-induced effects that are known to cause forbidden LO absorption, as observed by Venugopalan *et al.*²¹ in boron impurified $\text{Cd}_{0.9}\text{Mn}_{0.1}\text{Te}$ samples.

Above the transition pressure, a continuum beginning at 135 cm^{-1} is observed at all pressures. This indicates the existence of a light-induced shallow donor state with an ionization energy of 17 meV, which might be the Te donor associated with the L minima, which as mentioned above is expected to have an ionization energy of around 20 meV.²⁰ The ionization energy of this donor decreases slightly with applied pressure to 15 meV at 71 kbar.

As in the case of the sulfur DX center in InP (Ref. 6) we can estimate the energy of the Te DX level in GaSb at zero pressure relative to the conduction-band minimum, from the transition value of 27.8 ± 2.6 kbar. Chadi and Chang²² proposed that the pressure derivative of the DX level should be the same as that of the conduction band averaged over all k space since it is a localized state. The average is estimated using the expression proposed by those authors,²²

$$dE_{CB}/dP = [dE(\Gamma)/dP + 3 dE(X)/dP + 4 dE(L)/dP]/8.$$

We use $dE(\Gamma)/dP = 14.5 \pm 0.3 \text{ meV/kbar}$, $dE(X)/dP = -1.4 \pm 0.6 \text{ meV/kbar}$,²³ and $dE(L)/dP = 5 \pm 0.3 \text{ meV/kbar}$ (Ref. 24) to obtain $dE_{CB}/dP = 3.0 \pm 0.4 \text{ meV/kbar}$. This implies that the DX level approaches

the conduction-band minimum at Γ at the rate of $dE(\Gamma)/dP - dE_{CB}/dP = 11.7 \pm 0.7 \text{ meV/kbar}$ and that at zero pressure, the DX level energy is 325 meV above the conduction band. Furthermore, it was estimated in Ref. 25 that the DX level should be located 25 meV below the shallow donor energy in order for the sample to turn 90% transparent. Subtracting this correction to our total gives us $300 \pm 70 \text{ meV}$ as the position of the Te DX level above the conduction band at zero pressure.

Based on studies of sulfur-related DX centers, it has been suggested that these levels occur at the same energy in GaSb, GaAs, and InP, when the conduction-band offset energies among these compounds are taken into account.^{6,15} Similar calculations can now be performed for the Te DX center in $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$, $\text{Al}_x\text{Ga}_{1-x}\text{As}$, and $\text{GaAs}_{1-x}\text{P}_x$ alloys.^{1-3,26}

The band offset has been measured or calculated directly only among heterostructures of the GaSb/ $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ system.²⁷ For $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$, the binding energy of the Te DX has been reported to be $E_0 = 0.060 \text{ eV}$ for $x = 0.4$, when the band gap is $1.32 \pm 0.01 \text{ eV}$.²⁸ The valence-band offset of $\text{Al}_x\text{Ga}_{1-x}\text{Sb}/\text{GaSb}$ heterostructures at any composition can be calculated from the experimental fit of Menéndez *et al.*²⁷ as $0.18 \pm 0.01 \text{ eV}$ for $x = 0.4$, corresponding to a conduction-band offset of $0.33 \pm 0.02 \text{ eV}$. Assuming that the DX -center energies of the same group-VI impurity are indeed equal with respect to the vacuum level, one would expect the Te DX center to be found at $(0.33 \pm 0.02) - (0.06 \pm 0.01) \text{ eV} = 0.27 \pm 0.03 \text{ eV}$ above the GaSb conduction band, an estimation that compares very well with our present result of $0.3 \pm 0.07 \text{ eV}$. In Table I, we list the energy of Te DX center with respect to the bottom of the conduction band of GaSb, and the parameters used to determine it.

The band offset among GaSb/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and GaSb/ $\text{GaAs}_{1-x}\text{P}_x$ heterostructures may be obtained indirectly from the band offsets between these two alloys and GaAs, and that between GaAs and GaSb, all of which are known.²⁹⁻³¹ This information is listed in Table I to find the energy positions of the Te DX center in these alloys, where it can be seen that they coincide within the reported experimental uncertainties. This exercise certainly does show the tendency to line up in energy expected for the DX levels. Hence, the Te-related DX centers appear to follow the same dependence as the S DX centers in III-V compounds.

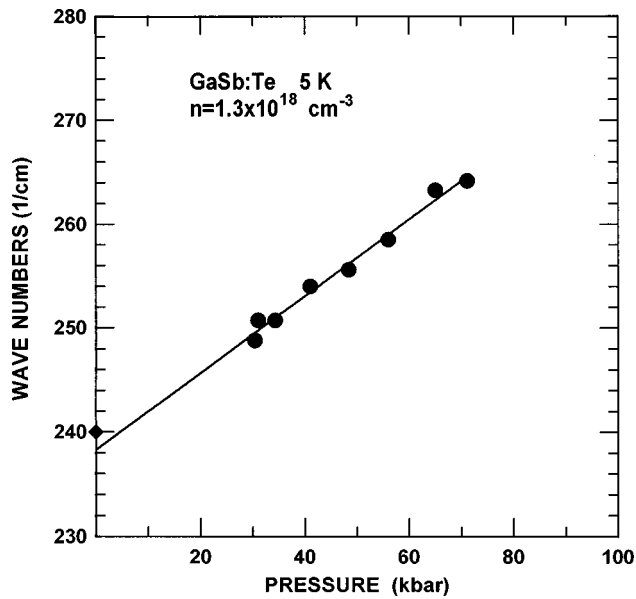


FIG. 2. Observed hydrostatic pressure dependence of the LO of GaSb, full circles. Full diamond, expected position of the LO phonon at liquid-helium temperatures. Straight line, least squares fit.

A recent theoretical calculation by Park and Chadi³³ predicts that Te should form *DX* centers in GaSb. This result is expected from two models: the broken-bond *DX* (BB-*DX*) of C_{3v} symmetry model and a model called cation-cation bonded *DX* (CCB-*DX*), which they claim may apply mainly for the sulfur *DX* donors. They calculate for the Te *DX* binding energies 70 and 210 meV above the conduction band, from the BB-*DX* and CCD-*DX* models, respectively. Comparison with the experimental binding energy 300 ± 70 meV obtained in this work for the Te *DX* donor favors a CCB-*DX* character for this center.³³

In Fig. 2, a plot of the observed bound phonon peak positions as function of the applied hydrostatic pressures is shown. The LO phonon should parallel very closely the pressure dependence of this bound phonon, which always appears very close in energy and at the low-energy side of the LO. From these data the resulting LO (bound phonon) pressure-dependent slope is estimated to be $d\omega_{LC}/dP = 0.38 \pm 0.04 \text{ cm}^{-1}/\text{kbar}$. From the slope we can determine the Grüneisen parameter that is used to describe the re-

sponse of the lattice vibrations to applied pressure or equivalently to isothermal compression, which is normally defined in terms of the TO optical phonon pressure derivative as

$$\gamma = B/\omega_{\text{TO}}(\delta\omega_{\text{TO}}/\delta P)_T = (\partial \ln \omega_{\text{TO}}/\partial \ln V)_T.$$

Here $B = 1/3(C_{11} + 2C_{12}) = 5.79 \times 10^5$ bar is the isothermal bulk modulus at low temperature and C_{11} and C_{12} are the elastic moduli in GaSb at 4.2 K.³² We obtain $\gamma_{\text{LO}} = 0.93 \pm 0.09$, a figure that is close to the almost “universal” value of 1.0 valid for many diamond and zinc-blende semiconductors.³⁴ As expected for the LO phonons it is smaller by an amount of 0.1–0.2 than the value derived from the pressure dependence of Raman scattering by TO phonons in GaSb of $\gamma_{\text{TO}} = 1.10 \pm 0.22$.³⁵

In summary, we have observed the transformation of Te shallow donors in GaSb into Te *DX* centers at hydrostatic pressures of 30.4 kbar and above. From the data, a transition pressure for this process is estimated to be 27.8 ± 2.6 kbar. The energy position of the Te *DX* center at zero pressure is calculated to be 300 ± 70 meV above the conduction band. The energies of Te-related *DX* centers appear to be consistent with the trend observed for S *DX* centers, that these are expected to line up in energy in all the III-V compounds in which they have been observed. The binding energy at zero pressure of the Te *DX* is well explained by the cation-cation bonded *DX*-center model of Park and Chadi.³³ At pressures where the Te shallow donor into *DX* center transformation has taken place we observe evidence of LO phonon absorption, which is normally forbidden in the IR. From the observed pressure dependence of this phonon, the LO Grüneisen parameter for this compound is calculated to be $\gamma_{\text{LO}} = 0.93 \pm 0.09$.

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