Hydrogen in compound semiconductors

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Hydrogen can be inadvertently introduced at any of several steps in the fabrication of optoelectronic devices. The most common consequence of hydrogenation is the passivation of dopant impurities, which leads to a decrease in the electrical conductivity of the material. The most successfully applied experimental technique for directly determining the involvement of hydrogen has been infrared-absorption local vibrational mode (LVM) spectroscopy. Examples of LVM spectroscopy of hydrogen-related complexes are given for the compound semiconductors GaP, ZnSe, GaN, GaAs, and AlSb. Recent studies have utilized large hydrostatic pressures to probe the vibrational properties of hydrogen-related complexes. © *1999 American Vacuum Society.* [S0734-2101(99)03104-8]

I. INTRODUCTION

Since the discovery of hydrogen passivation of acceptors[1] and donors[2] in GaAs, a great deal of research has been performed on hydrogen in compound semiconductors. In this article, recent results of local vibrational mode (LVM) spectroscopy of hydrogen-related complexes in compound semiconductors are reviewed. LVM spectroscopy is a useful technique for determining the microscopic structure of impurities and defects in semiconductors.[3,4] Hydrogen LVMs can be unambiguously identified through the substitution of deuterium, which reduces the LVM frequency by a factor of approximately $\sqrt{2}$. The LVM frequencies and the isotopic frequency ratio $r=\nu_H/\nu_D$ provide information about the bonding and position of the hydrogen.[5]

To date, a large number of hydrogen-related complexes have been discovered in III–V semiconductors. C–H complexes in GaAs have been intensively studied, both theoretically[6] and experimentally,[7] over the past five years. The four isotope combinations of these complexes (^{12}C–H, ^{13}C–H, ^{12}C–D, ^{13}C–D) each have four modes—one stretch (A_1), one longitudinal (A_1), and two transverse (E^- and E^+)—resulting in 16 LVMs, all of which have been observed experimentally. In addition, the C_{As}–C_{As} split interstitial pair can be passivated, resulting in the formation of $(C_{As})_2H$ and $(C_{As})_2H_2$ complexes.[8,9] C–H complexes have also been discovered in AlAs (Ref. 10) and GaP.[11]

Group VI donor–hydrogen complexes in GaAs give rise to sharp infrared absorption peaks due to hydrogen and deuterium stretch and wag modes.[12,13] In these complexes, hydrogen is believed to reside in an antibonding orientation. Pajot and Song[14] have observed numerous infrared absorption peaks between 2940 and 3500 cm^{-1} in oxygen-doped GaAs which are attributed to N–H and O–H stretch modes. Although hydrogen has long been suspected to form interstitial H_2 molecules in semiconductors, H_2 molecules have only recently been observed in GaAs by Raman spectroscopy.[15]

In this article, acceptor-hydrogen complexes in the compound semiconductors GaP, ZnSe, and GaN are described. In addition, recent discoveries involving hydrogen LVMs under pressure in GaAs and AlSb are reviewed.

II. EXPERIMENTAL TECHNIQUES

A. Fourier transform infrared spectroscopy

Midinfrared absorption spectra were obtained with a Bomem DA8 vacuum Fourier transform spectrometer with a KBr or CaF_2 beamsplitter. The samples were kept at a temperature of 9 K in a Janis liquid-helium cryostat with ZnSe windows. The instrument resolution was varied from 0.5 to 2 cm^{-1}, such that all peaks were fully resolved. Unless stated otherwise, spectroscopic data were obtained at or near liquid-helium temperatures (4–15 K). High-pressure measurements were performed in diamond anvil cells with N_2 as a pressure-transmitting medium.

B. Methods of hydrogenation

Hydrogen can be introduced into a sample by boiling in water, electrolysis, implantation, exposure to a hydrogen plasma, or contamination during the growth process.[5] In general, the omnipresence of hydrogen makes contamination with the ''simplest element'' difficult to avoid. In semiconductors grown by metalorganic chemical vapor deposition (MOCVD) the hydrogen may originate from the metalorganic molecules and the carrier gas (Secs. IV and V). To obtain acceptor–hydrogen complexes in GaP (Sec. III) and GaAs (Sec. VI), a hydrogen plasma was used. Finally, in the case of AlSb (Sec. VII), annealing in a hydrogen ambient was used as a method of bulk passivation.

C. Hydrogen plasma

Exposure to a hydrogen plasma is a common method of introducing atomic hydrogen into semiconductors to a depth of a few microns. The first hydrogen plasmas used for semiconductor passivation were produced in glow discharge tubes,[16] in which a dc bias of several hundred volts is applied between a metal anode and the sample, which acts as the cathode. Energetic electrons ionize hydrogen molecules and the resultant protons travel toward the sample with a steady

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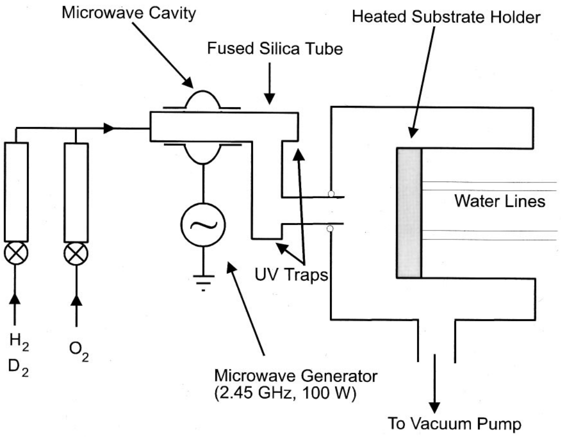

FIG. 1. Schematic diagram of a remote hydrogen plasma system (from Ref. 17).

current of several mA. A disadvantage of this simple technique is that the protons impinge on the sample surface with energies of several hundred eV, resulting in significant bombardment damage.

If an alternating electric field is used, however, the protons arrive at the surface with energies of only a few eV. The sample is typically located downstream from the radio frequency plasma to minimize charged particle bombardment damage. In a remote hydrogen plasma system,[17] shown in Fig. 1, hydrogen (or deuterium) and trace amounts of oxygen flow into the microwave cavity. Oxygen is used to suppress hydrogen recombination on the chamber walls, thereby increasing the fraction of atomic hydrogen.[17,18] The pressure in the chamber is kept at 2 Torr and the flow rates for the H_2 and O_2 are 50 and 0.3 sccm, respectively. The right-angle bends in the silica tube isolate the sample from ultraviolet (UV) radiation and charged particles.

Exposure to the low energy ions and neutral atoms introduces a subsurface layer of hydrogen which diffuses into the semiconductor. The concentration of the hydrogen near the surface depends on the hydrogen flux, surface absorption, diffusion rate, and the rate of recombination and desorption into H_2.

III. HYDROGEN IN GaP

For group II acceptor–hydrogen complexes in GaAs,[2] InP,[19] and GaP,[20] results from LVM spectroscopy show conclusively that hydrogen binds to the host anion in a bond-centered orientation, along a [111] direction, adjacent to the acceptor. By measuring overtones of hydrogen LVMs in InP, Darwich *et al.*[19] have determined the anharmonicity of the hydrogen potentials. As the atomic number of the group II acceptor increases from Be to Cd, the stretch mode frequency and isotopic frequency ratio $r=\nu_H/\nu_D$ increase.

The increase in the hydrogen LVM frequency can be described empirically by considering the equilibrium bond lengths of the diatomic molecules BeH, ZnH, and CdH. The *compression factor* is defined

$$\Delta = d(X-H)+d(Y-H)-d_{nn}, \tag{1}$$

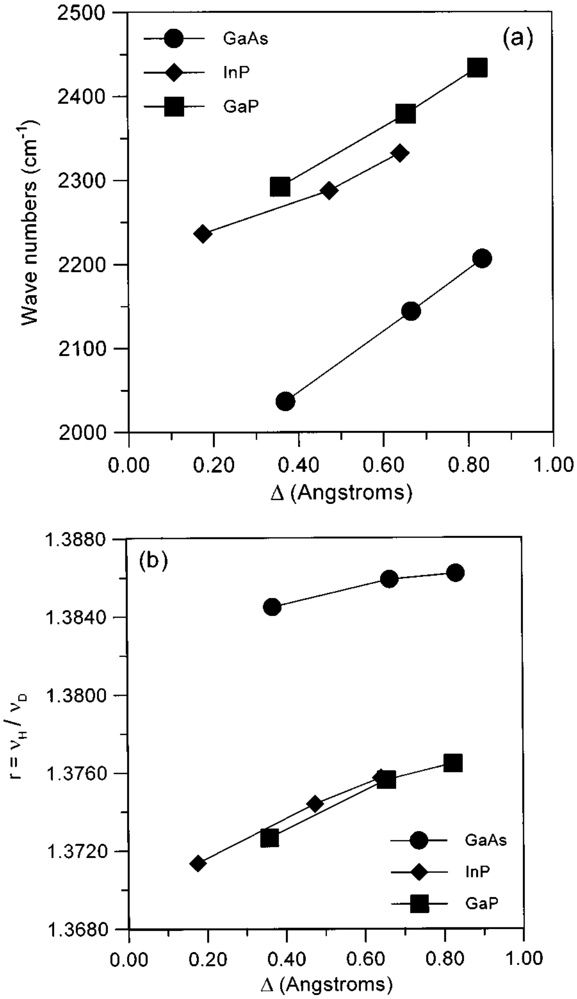

FIG. 2. (a) Vibrational frequencies and (b) isotopic frequency ratios *r* of group II–hydrogen complexes in GaAs, InP, and GaP.

where X is Be, Zn, or Cd, Y is P or As, $d(X-H)$ and $d(Y-H)$ are equal to the molecular bond lengths, and d_{nn} is the nearest neighbor lattice distance, given by

$$d_{nn}=\sqrt{3}a/4, \tag{2}$$

where a is the lattice constant. This simple model does not account for the distribution of charge between the $X-H$ and $Y-H$ bonds or the influence of other atoms in the lattice.

Δ is a relative measure of how much the bonds are compressed. As Δ increases, the LVM frequency and r value increase. Figure 2 shows the LVM frequencies and r values as a function of Δ for acceptor–hydrogen complexes in GaAs, GaP, and InP. For GaAs and GaP, the LVM frequencies vary linearly with Δ. The r values for GaP and InP lie on the same curve, apparently as a result of the similarity of the complexes. The compression of dopant-hydrogen bonds has been studied more directly through the application of hydrostatic pressure (Sec. VI).

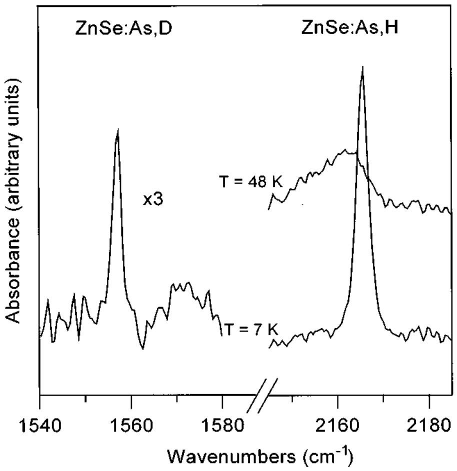

FIG. 3. Infrared absorption peaks of As–D and As–H complexes in ZnSe.

IV. HYDROGEN IN ZnSe:As

A. Introduction

ZnSe showed early promise as a material for blue laser diodes, with nitrogen as the preferred *p*-type dopant.[21,22] LVM spectroscopy of MOCVD-grown ZnSe:N revealed the presence of N–H complexes.[23,24] Arsenic, which replaces a host selenium atom, has also been investigated as a possible shallow acceptor.[25] The incorporation of hydrogen in arsenic- and MOCVD-grown ZnSe has been studied by secondary ion mass spectrometry (SIMS).[26] The hydrogen incorporation in ZnSe:As increases strongly when hydrogen is used as a carrier gas instead of nitrogen, as discussed next.

B. Experiment

A ZnSe:As sample that was grown with hydrogen as a carrier gas has an infrared absorption peak at 2165.6 cm^{-1} at a sample temperature of 7 K (Fig. 3).[27] When nitrogen is used as a carrier gas, the same peak is present, but its area is reduced by a factor of 14, in good agreement with SIMS measurements.[26] In the case of the nitrogen carrier gas, the hydrogen most likely originates from the metalorganic precursors. The sample that was grown with deuterium as a carrier gas has an absorption peak at 1557.1 cm^{-1}, along with the hydrogen-related peak at 2165.6 cm^{-1} (Fig. 3). The isotopic frequency ratio is $r=\nu_H/\nu_D=1.3908$. The area of the hydrogen-related peak is approximately three times that of the deuterium-related peak. Previous SIMS measurements of the samples show $[H]=6\times10^{18}\,\mathrm{cm}^{-3}$ and $[D]=1\times10^{18}\,\mathrm{cm}^{-3}$.[26] These results suggest that most of the hydrogen incorporation does not come directly from the carrier gas but, rather, from the metalorganic molecules.

C. Bond-centered model

Since the frequency of the ZnSe:As,H mode is similar to that of the AsH_3 bond-stretching mode frequency (2116 cm^{-1}),[28] it is likely that the hydrogen binds directly to the arsenic acceptor. In several respects, the As–H complex in ZnSe is remarkably similar to the Zn–H complex in GaAs.[2] In GaAs, zinc is an acceptor which occupies a substitutional gallium site. Hydrogen passivates zinc by attaching to a *host* arsenic atom, in a bond-centered orientation, adjacent to the zinc *acceptor*. In ZnSe:As the hydrogen attaches to the arsenic *acceptor*, in a bond-centered orientation, adjacent to the *host* zinc atom (Fig. 4). The stretch mode frequency of the GaAs:Zn,H complex is 2146.0 cm^{-1} at a temperature of 6 K, and the isotopic frequency ratio is $r=1.3860$. The fact that the *r* values and LVM frequencies of the two complexes are very similar lends further support to the bond-centered model.

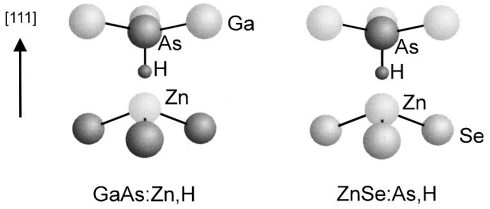

FIG. 4. Bond-centered models for GaAs:Zn,H and ZnSe:As,H complexes.

V. HYDROGEN IN GaN:Mg

A. Introduction

The development of blue light-emitting diodes (LEDs)[29] and laser diodes[30] has focused a great deal of research activity on GaN-based III–V nitrides. The band gaps of $In_xGa_{1-x}N$ alloys cover a wide spectral range, from red (InN) to UV (GaN), making this alloy system ideal for numerous optoelectronic applications.[31]

MOCVD is the dominant growth technique for III–V nitride devices, with Mg the most common *p*-type dopant. As a result of hydrogen passivation during growth, as-grown GaN:Mg is semi-insulating. It was shown empirically that low energy electron beam irradiation (LEEBI)[32] or thermal annealing at temperatures above 600 °C in a N_2 ambient[33] was required to activate the Mg acceptors. Since thermal annealing had been shown to dissociate acceptor–hydrogen complexes in numerous other semiconductors,[1,2] it was assumed that Mg–H complexes were formed in GaN as well. It required infrared spectroscopy, however, to positively identify the Mg–H complexes.[34] In GaN grown by molecular beam epitaxy (MBE) the lack of hydrogen enables one to grow *p*-type GaN:Mg without LEEBI or thermal annealing.[35]

B. N–H model

Theoretical calculations predict that hydrogen attaches to a nitrogen atom in an antibonding orientation (Fig. 5) in the Mg–H complex,[36] in stark contrast to acceptor–hydrogen complexes in non-nitride semiconductors. This difference can be attributed to the ionicity of the Ga–N bond, in which there is no local maximum of the charge density at the bond center. In the strongly covalent Ga–As and Si–Si bonds, on the other hand, there is a maximum in the charge density which attracts the proton to the bond-centered location.

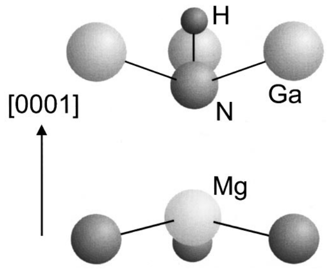

FIG. 5. Antibonding model for the Mg–H complex in GaN.

The predicted stretch mode frequency of hydrogen in the Mg–H complex is 3360 cm^{-1},[36] which is similar to that of NH_3 (3444 cm^{-1}). The stretch mode frequency was experimentally observed at 3125 cm^{-1} in 4-μm-thick epilayers of MOCVD-grown GaN:Mg.[34] This frequency agrees quite well with the theoretical prediction of 3360 cm^{-1} and is similar to the stretch mode frequencies of N–H complexes in GaAs (Ref. 14) and ZnSe.[23,24] Upon annealing, the peak at 3125 cm^{-1} decreases by a factor of 2 (Fig. 6) and is correlated with an increase in the conductivity. Annealed samples that are exposed to a remote deuterium plasma show a deuterium stretch mode peak at 2321 cm^{-1}. The isotopic frequency ratio is $r=\nu_H/\nu_D=1.346$, which is very similar to that of NH_3 ($r=1.342$), lending further support to the N–H model. Whether the hydrogen resides in an antibonding or bond-centered position, however, has not yet been determined experimentally.

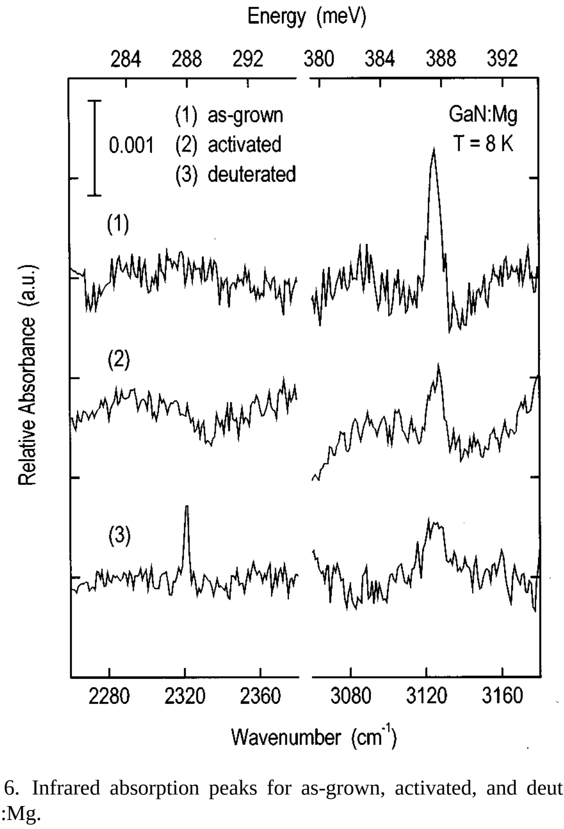

FIG. 6. Infrared absorption peaks for as-grown, activated, and deuterated GaN:Mg.

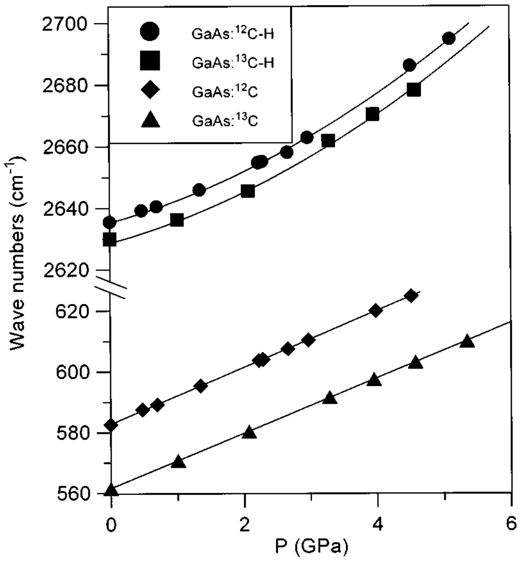

FIG. 7. GaAs:C,H and GaAs:C LVMs as a function of pressure.

VI. GaAs LVMs UNDER PRESSURE

The application of hydrostatic pressure is an excellent tool for probing the electronic and vibrational properties of defects in semiconductors.[37–39] Only recently has this experimental probe been utilized to investigate hydrogen-related complexes.

A. GaAs:C,H

In the GaAs:C,H complex, the hydrogen attaches directly to the carbon acceptor, in a [111] bond-centered orientation, adjacent to a host gallium atom.[6,7] At atmospheric pressure and liquid-helium temperatures, the ^{12}C–H and ^{13}C–H stretch modes have frequencies of 2635.2 and 2628.5 cm^{-1}, respectively.[7]

The peak positions of the ^{12}C–H, ^{13}C–H, ^{12}C, and ^{13}C modes are plotted as a function of pressure in Fig. 7. Since the $^{12}C_{As}$–H and $^{13}C_{As}$–H stretch mode frequencies only differ by 0.3%, the difference in pressure dependence cannot be resolved experimentally. The plots of the hydrogen stretch modes as a function of pressure are nonlinear, with a positive curvature. The substitutional carbon LVMs, however, vary linearly with pressure.

B. GaAs:S,H

In group VI donor–hydrogen complexes, the hydrogen is believed to bond with a host gallium in a [111] antibonding orientation.[15] Since the hydrogen is isolated from the donor, its LVM frequency is very insensitive to the donor species, only varying ~10 cm^{-1} from S to Te. The pressure dependence of the S–H stretch and wag modes and the S–D wag mode was measured. The S–D stretch mode was too weak to be detected in the diamond anvil cell sample. The frequencies of the stretch and wag modes are plotted as a function of pressure in Fig. 8. The S–H and S–D modes vary linearly

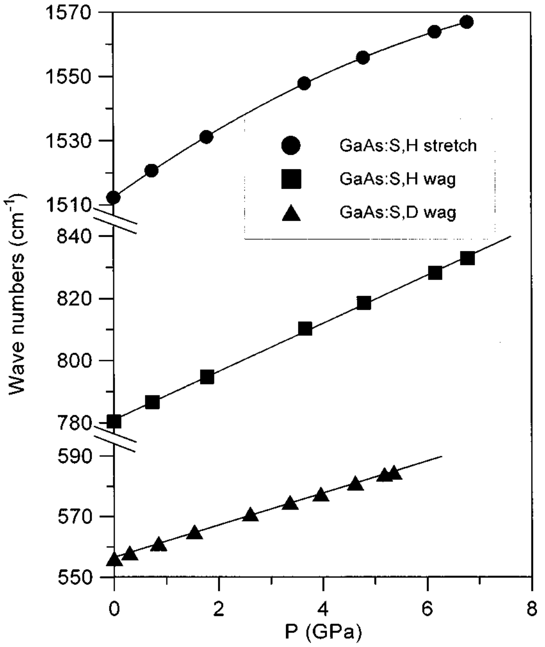

FIG. 8. GaAs:S,H and GaAs:S,D LVMs as a function of pressure.

with pressure. The plot of the hydrogen stretch mode as a function of pressure is nonlinear, with a negative curvature.

C. Summary

The pressure dependence of LVM frequencies in GaAs is a strong function of local environment.[40] As in the case of AlSb:^{12}C (Ref. 41) and GaAs:^{28}Si,[39] the ^{12}C and ^{13}C LVM frequencies vary linearly with pressure. The pressure dependent shifts of the ^{12}C–H and ^{13}C–H stretch modes have positive curvatures, while the shift of the S–H stretch mode has a negative curvature. This may be related to the fact that in the bond-centered C–H complex, the hydrogen is compressed between the carbon acceptor and one gallium host atom, whereas in the S–H complex, the hydrogen occupies an interstitial position and is not crowded by neighboring atoms. In the future, pressure may be utilized to differentiate between bond-centered and antibonding configurations.

VII. AlSb:Se,H UNDER PRESSURE

At liquid-helium temperatures, hydrogenated AlSb:Se has stretch mode peaks at 1608.6 and 1615.7 cm^{-1}, whereas the Se–D mode has only one stretch mode peak at 1173.4 cm^{-1}.[42] In addition, there is a small Se–H peak at 1606.3 cm^{-1}. Hydrogenated and deuterated AlSb:Te have only one stretch mode peak each, at 1599.0 and 1164.4 cm^{-1}, respectively. The anomalous splitting of the Se–H peak may be explained in terms of a resonance between the stretch mode and combination modes involving extended lattice phonons and a wag mode harmonic.[43] Hydrostatic pressure was utilized to change the resonance conditions between local and extended modes. The peak positions are plotted in Fig. 9.

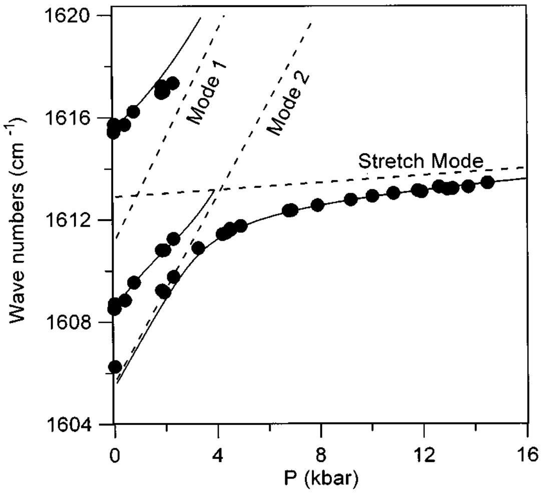

FIG. 9. Se–H peak frequencies in AlSb as a function of pressure.

To explain the existence of three peaks, it was proposed that the stretch mode interacts with two ''unknown'' modes, 1 and 2. It should be noted that the calculated AlSb optical phonon density of states has a sharp peak at $\omega_p = 290\,\mathrm{cm}^{-1}$.[44] The experimentally measured frequency of the $N=3$ and $N=4$ wag mode harmonics (Γ_1) are $\omega_{\mathrm{wag},3} = 1032\,\mathrm{cm}^{-1}$ and $\omega_{\mathrm{wag},4} = 1316\,\mathrm{cm}^{-1}$, respectively.[42] The combination modes may therefore be given by

$$\omega_1 = 2\omega_p + \omega_{\mathrm{wag},3} \sim 1612\ \mathrm{cm}^{-1}, \tag{3}$$

$$\omega_2 = \omega_p + \omega_{\mathrm{wag},4} \sim 1606\ \mathrm{cm}^{-1}, \tag{4}$$

which are very nearly degenerate with the Se–H stretch mode.

The pressure dependence of the peaks can be understood qualitatively as follows: the stretch mode interacts primarily with combination mode 1 and splits into two branches. The low-frequency branch then interacts with mode 2, with a smaller coupling energy. The anticrossing between the three modes yields three infrared active peaks at pressures of ~2 kbar. For higher pressures, only the lowest branch, peak 0, is ''LVM like.'' Pressure was used to decouple the stretch mode from modes 1 and 2.

VIII. CONCLUSIONS

Hydrogen in compound semiconductors continues to be an important topic, both from a scientific and technological viewpoint. Recent measurements have utilized temperature and hydrostatic pressure as experimental probes of hydrogen LVMs. From the shifts of the LVM frequencies, information can be obtained about the interaction between hydrogen and impurity/host atoms. In the future, these techniques may be used to provide clues about the location of hydrogen atoms within complexes as well as the nature of LVM–phonon interactions.

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