Temperature dependence of the infrared dielectric function and the direct band gap of InSb from 25 to 800 K

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In experiment, the infrared dielectric function of InSb in the region of the direct band gap at temperatures from 77 to 725 K using Fourier-transform infrared spectroscopic ellipsometry is determined. At the highest temperatures, the free carrier concentration due to thermally excited electron-hole pairs becomes very large and the Fermi level is above the conduction band minimum. The observed band gap increases again at 600 K (Burstein-Moss shift).

Theoretically, the temperature dependence of the chemical potential μ for an ideal intrinsic semiconductor (InSb) at fixed temperatures is calculated by using Polylogarithm forms of FD integrals. It is known that at absolute zero, the chemical potential (μ) is equal to the Fermi energy (ε_F). μ versus T is plotted for Degenerate and Non-Degenerate case (this calculation assumes parabolic bands, a constant band gap, and constant effective masses). On comparing both graphs we can see at higher temperature degenerate graph goes up (deviate up) but for non-degenerate case, it remains linear. Due to the small electron to hole mass ratio, the optical activation energy (OAE, i.e., the experimental band gap measured with transmission or ellipsometry measurements) is almost the same as the chemical potential, once μ is larger than the band gap (above about 400 K). It is apparent that there is a thermal Burstein-Moss shift for temperatures above 400 K, because the chemical potential and the OAE are larger than the intrinsic band gap.

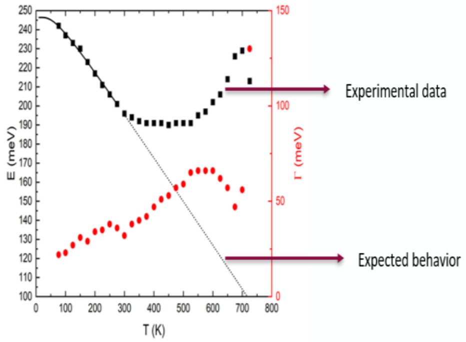

Fig1: Direct band gap $\boldsymbol{E_0}$ (▪) and broadening (·) of InSb as a function of temperature. (Experimental Result)

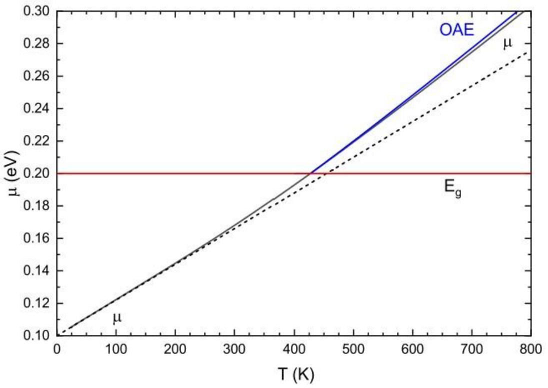

Fig 2: Chemical potential for intrinsic InSb v/s temperature in the degenerate (solid) and non-degenerate (dotted) case. The red horizontal line shows the band gap of 0.2 eV. The blue line shows the optical activation energy (OAE, i.e., the experimental band gap)

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Supplementary Pages (Optional)

In Experimental work, the temperature dependence of the complex pseudo-dielectric function of bulk InSb (100) near the direct band gap was measured with Fourier-transform infrared ellipsometry between 30 and 500 meV at temperatures from 80 to 725 K in ultrahigh vacuum. Using the Jellison-Sales method for transparent glasses, the thickness of the native oxide was found to be 25±5 ˚A, assuming a high-frequency dielectric constant of about 3.8 for the native oxide. After this surface correction, the dielectric function was fitted with a Herzinger-Johs parametric semiconductor model to determine the band gap and with a Drude term to determine the electron concentration and the mobility. We find that the band gap decreases from 230 meV at 80 K to 185 meV at 300 K, as expected from thermal expansion and a Bose-Einstein model for electron-phonon scattering renormalization of the band gap. Between 450 and 550 K, the band gap remains constant near 150 meV and then increases again at even higher temperatures, presumably due to a Burstein-Moss shift resulting from thermally excited electron-hole pairs. The broadening of the direct band gap increases steadily with temperature. (See Fig. (a))

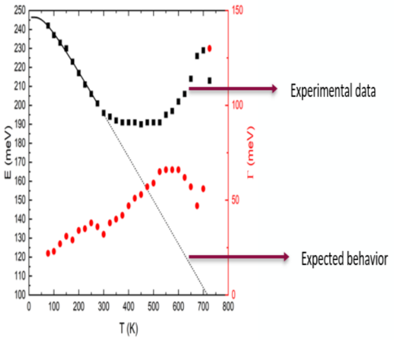

Fig: (a)

We described a theoretical model that is used to explain these experimental results.

For an undoped (intrinsic) semiconductor with parabolic bands, the electron and hole concentrations as a function of temperature T are given by,

$$n\,(T) = \frac{1}{4}\left(\frac{2m_0\, m_e k_B T}{\pi\hbar^2}\right)^{\frac{3}{2}} F_{\frac{1}{2}}\left(\frac{\mu - E_0}{k_B T}\right),\ p(T) = \frac{1}{4}\left(\frac{2m_0\, m_h k_B T}{\pi\hbar^2}\right)^{\frac{3}{2}} F_{\frac{1}{2}}\left(\frac{-\mu}{k_B T}\right)$$

where m_e and m_h are the effective density-of-states masses of the conduction and valence bands and $\hbar$ is the reduced Planck's constant. μ is the chemical potential, and E_0=0.2 eV is the direct band gap, which we have assumed to be constant. We also assumed constant effective masses. For sufficiently low temperatures, the argument of the Fermi-Dirac integral $F_{1/2}$ becomes very large, and the Fermi integral can be expanded into essentially using Maxwell-Boltzman statistics to describe the electron and hole populations.

$$\mu \approx \frac{E_0}{2} + \frac{3k_B T}{4}\, ln\left(\frac{m_h}{m_e}\right), \qquad \mu \approx 2\left(\frac{m_0 k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} (m_e m_h)^{\frac{3}{4}} \exp\left(-\frac{E_0}{2k_B T}\right)$$

For InSb, these expressions can be used up to 300 K, but deviations become noticeable at higher temperatures. Above 300 K, we must use the exact definition of the Fermi-Dirac integral.

$$F_{\frac{1}{2}}(\eta) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{y}}{\exp(y-\eta)+1} dy$$

We evaluate the Fermi-Dirac integrals $F_{(1/2)}$ by noting their connection with polylogarithm functions $L_{i(n+1)}$, which were calculated using the polylog () function in MATLAB.

$$F_{\frac{1}{2}}(\eta) = -L_{i_{n+1}}(-e^{\eta})$$

In an intrinsic semiconductor, electrical neutrality requires that n (T)=p (T). For a given temperature T, we therefore plot n and p as a function of μ. The intrinsic chemical potential is found at the location where the two lines cross. As an example, we show the electron and hole concentrations as a function of the chemical potential at 300 K. The two curves cross at the intrinsic chemical potential of 168 meV at 300 K. (See Figure (b)).

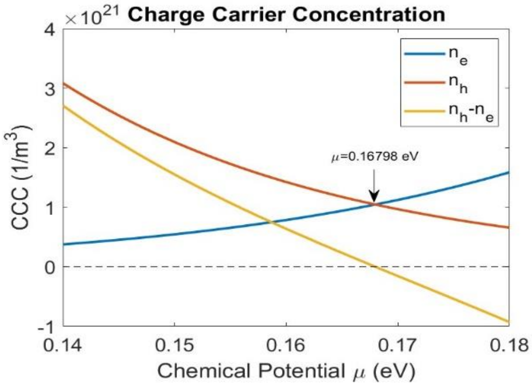

Fig: (b)

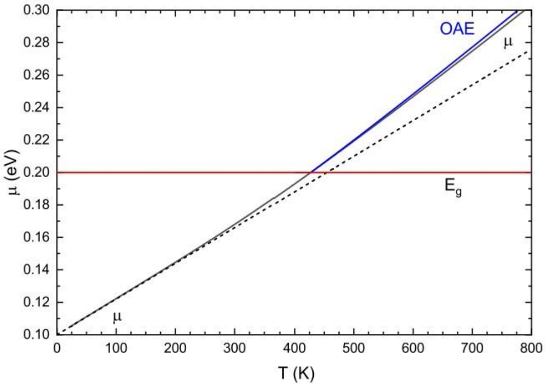

Fig: (c)

We then vary the temperature from 25 to 800 K and calculate the intrinsic chemical potential at each step. Below 25 K, the dependence of the carrier concentration on the chemical potential is very weak and we therefore we use non-degenerate limit to calculate the chemical potential below 25 K. The chemical potential increases linearly with temperature in the non-degenerate limit (dashed). The degenerate chemical potential (solid) increases super linearly with temperature and is somewhat larger than for the non-degenerate limit. The two curves start to separate above 200 K. Near 400 K, the chemical potential is equal to the band gap. This means that the Fermi level crosses over into the conduction band, making InSb fully degenerate. (See Figure (c)). The optical activation energy (OAE, i.e., the experimental band gap measured with transmission or ellipsometry measurements) is given by;

$$E_A = max\left[E_{0,}E_0 + \left(1+\frac{m_e}{m_h}\right)(\mu - E_{0)}\right]$$

Due to the small electron to hole mass ratio, the OAE is almost the same as the chemical potential, once μ is larger than the band gap (above about 400 K). The OAE is also shown in Fig.(c). It is apparent that there is a thermal Burstein-Moss shift for temperatures above 400 K, because the chemical potential and the OAE are larger than the intrinsic band gap. This Burstein-Moss shift is about 0.1 eV at 750 K, which is similar to the difference between the experimental band gap (■) and the dotted line in Fig. (a).