Bandgap vs Temp an Inquiry and an Exercise

In lecture 6, slide 11 we examined the effect of temperature on the absorption edge and corresponding bandgap of vitreous As2S3. (Figure from Feltz, p 380). One student asked about the origin of this temperature dependence, so let us explore the question together through an exercise.

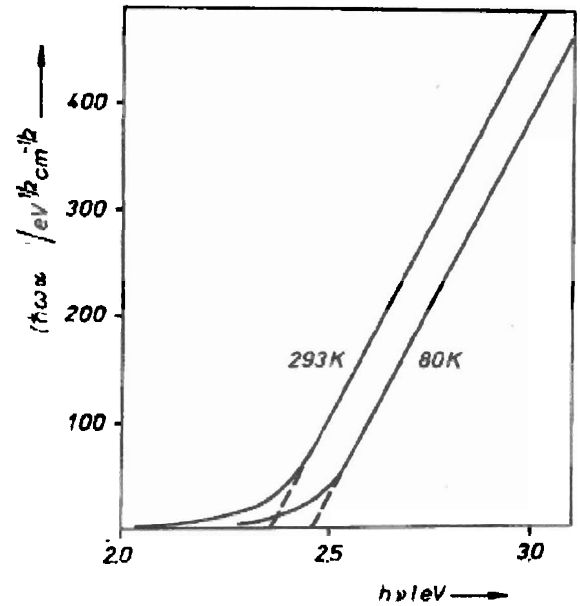


Fig. 4.44. Plot of the absorption edge for vitreous As_2S_3 at 293 K and 80 K (according to [4.280]).

a) Estimate the temperature dependence of the bandgap (dE_g/dT) for this material and compare it to that of the common III/V optoelectronic material GaAs (Kasap p 149 gives -4.5 x 10^{-4} eV/K for GaAs semiconductor or calculate your own using http://ecee.colorado.edu/~bart/book/eband5.htm).

$$\frac{dE_g}{dT} \approx \frac{\Delta E_g}{\Delta T} = \frac{0.1\,\text{eV}}{213\,^\circ\text{K}} = 4.7\times10^{-4}\ \text{eV/K}$$

Remarkably similar!

b) One explanation for the temperature dependence of the bandgap could be simply from the thermal expansion of the material and the resulting change in bandgap with increased atomic spacing. In this case the temperature dependence of the bandgap can be estimated from the dependence on lattice spacing (a) and the linear thermal expansion (α) using: $dE_g/dT = a*dE_g/da * \alpha$. Show how we obtain this equation.

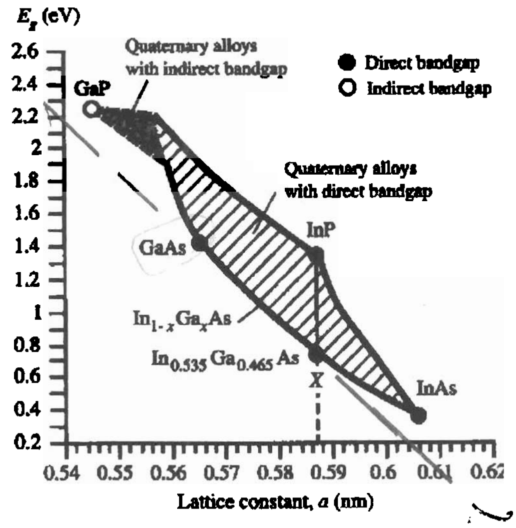
$$\frac{dE_g}{dT} = \frac{\partial E_g}{\partial a}\cdot\frac{da}{dT} + \sum \frac{\partial E_g}{\partial \xi}\, d\xi/dT$$

other variables we ignore per assumption

$$= \left(\frac{\partial E_g}{\partial a}\right)\cdot a\left(\frac{1}{a}\frac{da}{dT}\right) = a\left(\frac{\partial E_g}{\partial a}\right)\alpha$$

c) Optoelelctronic engineers design their devices using bandgap vs lattice constant plots such as the one shown here (see Kasap, p 155). Use the plot to estimate the dE_g/da for GaAs.

$$\frac{dE_g}{da} \cong -\frac{2.2-0.2}{0.604-0.54} = -31.25\ \text{eV/nm}$$



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d) From the value of dE_g/da estimated above, calculate the estimated value of the dE_g/dT for GaAs. You will need the α value or an estimate of the same. (See e.g., http://www.ioffe.ru/SVA/NSM/Semicond/GaAs/thermal.html

How does your estimate compare to the dE_g/dT value for GaAs given in part a?

$a \frac{\partial E_g}{\partial a} = 0.56 nm \times 31.25 ev/nm = 17.5 ev$

$\alpha (GaAs, 100°C) = 5.7 \times 10^{-6}$ 1/K

$\frac{d}{dT} = -17.5 ev \times 5.7 \times 10^{-6}$ 1/K

$\approx -1.0 \times 10^{-4}$ ev/K

This is only ~ 21% of the observed dependence, See Note below.

e) For the As2Se3 glass, Felty and Meyers (1967) give a linear thermal expansion value of 20.7 x 10-6 /K. Use this value and repeat the calculation of part d, using the same dE_g/da found for GaAs. How does this estimate of the dE_g/dT compare with that calculated in part a?

use

$\frac{dE_g}{dT}(Ge_2Se_3) \cong a \frac{\partial E_g}{\partial a} \cdot \alpha (Ge_2Se_3 \text{ glass})$ (from GaAs)

$= -17.5 ev \times 20.7 \times 10^{-6}$ 1/K $= -3.62 \times 10^{-4}$ ev/K

AND This is 75% of the observed dependence,

How might we get an experimental measurement of the $\frac{dE_g}{da}$ for the Ge_2Se_3 glass?

Note: S. A. Lourenco¸et. al. provide an analysis of this issue of origin of T dependence of the bandgap in III/V materials and in their introduction state "The temperature dependence of the band-gap energy, in special, can be explained by the sum of two distinct mechanisms: the electron-phonon interaction and the lattice thermal expansion. The main contribution to the temperature dependence of the band-gap energy is attributed to electron-phonon interactions." Their overall conclusion is that "the thermal expansion contribution to GaAs, at room temperature, represents 21% of the total shift of the excitonic transition energy".

S. A. Lourenco, et. al. Brazilian Journal of Physics, vol. 34, no. 2A, June, 2004. Thermal Expansion Contribution to the Temperature Dependence of Excitonic Transitions in GaAs and AlGaAs available at: http://www.sbfisica.org.br/bjp/files/v34_517.pdf

For thermal expansion data on As2Se3 take a look at: E. J. FELTY and M. B. MYERS, Journal of the American Ceramic Society, Volume 50, Issue 6, pages 335–336, June 1967, "Thermal Expansion of Arsenic-Selenium Glasses".

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