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LOW-TEMPERATURE LIMIT OF GRÜNEISEN'S GAMMA OF GERMANIUM AND SILICON

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Gibbons[1] has measured the thermal expansion of Ge, Si, and InSb at low temperatures. Using these data and values of the heat capacity measured by various investigators, together with the Grüneisen relation,[2]

$$\gamma = \alpha V / \chi_T C_v, \tag{1}$$

he obtains a plot of γ vs T/Θ_∞ reproduced as the solid lines of Fig. 1. α is the volume coefficient of thermal expansion, V the crystal volume, χ_T the isothermal compressibility, and C_v the heat capacity at constant volume. This plot indicates an anomalous negative peak for the case of Si and InSb, but not for Ge over the range of temperatures investigated. Gibbons has indicated by the dashed lines an extrapolation of γ toward zero as T/Θ_∞ goes to zero. It is known that these materials with diamond-like structures reveal extraordinarily similar behavior in other lattice properties such as the temperature dependence of their Debye temperatures and even their lattice spectra.[3] It seemed, then, worth investigating this situation wherein a difference of behavior was observed. Sheard[4] discusses a way of obtaining high- and low-temperature limiting values of γ from a knowledge of the pressure dependence of the elastic constants of a solid, involving the averaging of a property over all the directions of a crystal. We have found a simple and quick method of obtaining the limiting value of γ as T approaches zero, from the following considerations. Derivation[2] of the relation (1) on the assumption that the Debye temperature is independent of temperature, which should be expected to be valid at very low temperatures, yields $-\gamma = d\ln\Theta / d\ln V$. It is possible to calculate the limiting value of the Debye temperature at 0°K from the values of the elastic constants, molar volume, and density of a material: de Launay[5] has prepared tables from which one can easily evaluate Θ_0 using the relation:

$$\Theta_0{}^3 = \frac{9N}{4\pi V}\left(\frac{h}{k}\right)^3\left(\frac{C_{44}}{\rho}\right)^{3/2}\frac{9}{18+\sqrt{3}}f(s,t), \tag{2}$$

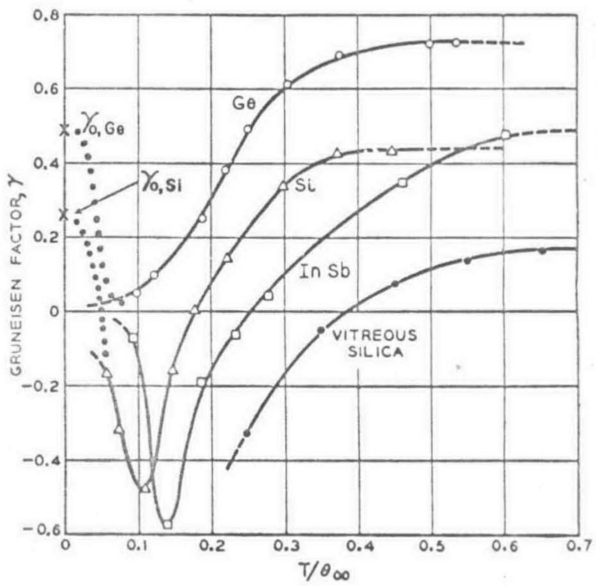

FIG. 1. Variation of Grüneisen factor with reduced temperature T/Θ_∞ for germanium ($\Theta_\infty = 400$°K), silicon ($\Theta_\infty = 674$°K), vitreous silica ($\Theta_\infty = 495$°K), and indium antimonide ($\Theta_\infty = 214$°K).[1]

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where

$$s=(C_{11}-C_{44})/(C_{12}+C_{44}),\quad t=(C_{12}-C_{44})/C_{44}.$$

N is the total number of atoms, V is the volume, ρ is the density, and the remaining symbols have their usual meanings. $f(s,t)$ is presented in tabular form. From reference 2 one can obtain

$$\frac{d\ln\Theta_0}{d\ln V}=\frac{1}{2}\frac{d\ln C_{44}}{d\ln V}+\frac{1}{6}+\frac{1}{3}\frac{d\ln f(s,t)}{d\ln V},$$

which can be evaluated using the tables and the known values of C_{ij} and $d\ln C_{ij}/d\ln V$ for Ge[6] and Si.[7] Term by term the results are, for Ge and Si,

$$\text{Ge:}\quad d\ln\Theta_0/d\ln V=-\gamma_0=-0.751+0.167+0.092=-0.492;$$

$$\text{Si:}\quad -\gamma_0=-0.490+0.167+0.073=-0.250.$$

Note that the third term, involving the interpolation in the table and arising from the change of elastic anisotropy and Poisson ratios with volume, is a relatively small correction for these materials. The values of γ_0 so obtained are indicated by $\times$'s on the $T/\Theta_\infty=0$ ordinate of Fig. 1. A possible interpolation of the data is indicated by a dotted line, whence the γ of Ge does exhibit the same behavior as that of Si and InSb. It seems probable that Gibbons' extrapolation given by the dashed line is incorrect in the case of Ge and that the similarity of behavior of Ga, Si, and InSb is preserved.

[1]D. F. Gibbons, Phys. Rev. 112, 136 (1958).

[2]See, for example, C. Kittel, Introduction to Solid-State Physics (John Wiley & Sons, New York, 1956), 2nd ed., pp. 153-155.

[3]J. C. Phillips, Phys. Rev. 113, 147 (1958).

[4]F. W. Sheard, Phil. Mag. 3, 1381 (1958).

[5]J. de Launay, in Solid-State Physics, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1956), Vol. 2, p. 219.

[6]H. J. McSkimin, J. Acoust. Soc. Am. 30, 314 (1958).

[7]J. C. Chapman, Masters thesis, Case Institute of Technology, Cleveland, Ohio (unpublished).