Study of Specific–Heat and Debye–Characteristic Temperature

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ABSTRACT

The study of specific heat in solids provides fundamental insights into lattice vibrations and electronic behavior, especially at low temperatures. The Debye model offers a theoretical framework to understand the lattice contribution to specific heat, introducing the Debye characteristic temperature () as a key parameter reflecting phonon dynamics and bonding strength. This work reviews the theoretical foundations of the Debye model, the temperature dependence of specific heat in metals, and methods to experimentally determine . By analyzing the low-temperature behavior of specific heat, both the lattice () and electronic () contributions can be separated, allowing for the evaluation of material properties such as sound velocity, thermal conductivity, and electron density of states. The Debye temperature emerges as a crucial indicator of a material's elastic and thermal characteristics, with significant implications for solid-state physics, materials science, and thermoelectric applications.

KEYWORDS

Specific Heat, Debye Temperature, Debye Model, Lattice Vibrations, Phonons, Low-Temperature Heat Capacity, Electron-Phonon Interaction, Solid-State Physic, Thermal Properties, Metals

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I. INTRODUCTION

The evaluation of specific-heat is possible only when the vibrational-frequencies in the lattice are completely determined. The specific-heat at constant volume C_v is given by

$$C_v = \left(\frac{\partial E}{\partial T}\right)_v \qquad \text{...(1)}$$

Where E is the total internal energy.

Looking into the development of theory of specific-heat, it becomes obvious that frequency-distribution function $g(v)$, plays an important role in dictating the contribution of vibrational modes to the thermodynamic properties. Once the frequency distribution function is known the lattice specific heat at constant volume C_v can be calculated from the following expression obtained from equation (1).

$$C_v = 3NK_B \frac{\int_0^{vm}\left(\frac{hv}{KBT}\right)^2 \cdot \frac{e^{hv}}{KBT}g(v)\partial v}{\left(\frac{e^{hv}}{KBT}-1\right)^2} \Big/ \int_0^{vm} g(v)\bullet \partial v \qquad \text{...(2)}$$

Where v_m is the maximum frequency, N the Avogadro's number. When converted to summation, convention suitable for computation, equation (2) becomes

$$C_v = 3NK_B \frac{\sum E\left(\frac{hv}{KBT}\right)^2 \cdot g(v)\partial v}{\sum g(v)\bullet \partial v} \qquad \text{...(3)}$$

Where $E(\frac{h}{K_BT})$ is the Einstein-function determined by

$$E(x) = -\frac{x^2 \bullet e^2}{[e^2-1]^2} \qquad \text{...(4)}$$

With $x = \left(\frac{hv}{K_B \bullet T}\right)$

Also, $\sum g(v) \bullet dv$ = Total number of frequencies considered. =3000

Hence equation (3) can be written for fee structure as

$$C_v = \frac{3NK_B}{3000} \bullet \sum E(x)g(v)\partial v \qquad \qquad ...(5)$$

The direct experimental determination of the frequency distribution function has been made possible only in a few cases, owing to various experimental difficulties. The most straight forward and direct method for determining $g(v)$ lies in determining the vibration frequency for a large number of points within the first Brillouin-zone. For this purpose first Brillouin-zone has been divided into 1000 miniature cells with sides one tenth of the length of the reciprocal lattice cell.

From the symmetry requirements of the lattice these 1000 points are reduced to 48 non-equivalent points including the origin of fcc metals. These points lie within 1/48th part of the Brillouin zone, which is irreducible under symmetry operations that leave the roots of secular determinant unchanged.

The calculation of the frequencies has been made for these non-equivalent points by solving secular determinants for values of wave-vectors, corresponding to these points. Each frequency is assigned a statistical weight according to the number of similar points associated with it. When probably weighted the vibration spectra corresponding to these non-equivalent points will present the complete vibration spectra for the solid and the frequency distribution function $g(v)$ can be obtained by use of Blackmann sampling technique.

For sampling purpose the entire frequency range is divided into a number of small intervals and all the frequencies lying within these intervals and entire with the proper statistical weights.

The contribution of each frequency Interval to the specific-heat is obtained by multiplying the Einstein's-function corresponding to the mid-point of the interval by its statistical weight for which the interval by obtained from the number of frequencies lying in the intervals The contribution of all such intervals when summed un give $\sum E(x)g(v)\partial v$ The lattice specific heat is then calculated by expression (5) above.

The sampling technique is useful only when the number of frequencies falling in each frequency internal is sufficiently large. For very low temperature i.e., below 20°k this technique becomes unreliable because the mesh of the points at low temperature becomes too coarse to give accurate values of C_v.

At these temperatures the contribution of the outer portion of the Brillouin zone to the specific beat gradually decreases and its value becomes increasingly dependent on the central part of the Brillouin zone and the dominant effect of the low frequency end of the spectrum is experienced below 20° K the modified Houstan's method elaborated by Betts et el can be used.

For theoretical evaluation of Debye-temperature $\theta_D = \frac{hv_m}{K_B}$ at different temperatures. We use the calculated values of C_v at different temperatures. For this purpose $(C_v - \frac{\theta_D}{T})$ is used and $\frac{\theta_D}{T}$ value corresponding to any value of C_v is obtained.

Therefore, the value of θ_D at different temperature are theoretically calculated. These θ_D values have been plotted as a function of temperature T and compared with the experimental values of θ_D.

TABLE
Values of electronic specific heat co-efficient Ye for fcc metals.

Metals	$\gamma_e \times 10^{-4} Cal \bullet mole^{-1} \bullet k^{-2}$	Reference
Transition metals		
Palladium	22.510	118
Thorium	19.000	125
Nickel	16.790	132
P-Block metals		
Aluminium	3.2203	133
Lead	3.0000	136
Noble metals		
Copper	1.652	104
Silver	1.531	104
Gold	1.651	104

II.   RESULTS AND DISCUSSION

Theoretical values of specific heat have been calculated for three noble metals (copper, silver, gold), three transition metals (palladium, thorium, nickel) and two p-block metals (aluminium, lead) all having fcc structure. Calculated values of specific heat are used to calculate the Debye characteristic temperatures of above metals. The calculated results are compared with the experimental values These are described in the following subsections.

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