

Measurements of Heat Capacity from Lattice Vibrations of Solids by Using Debye Model

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Abstract

Heat capacity is a measurable physical quantity that characterizes the ability of a body to store heat as its temperature changes, it is defined as the amount of heat that changes the temperature of the body at the given conditions. The objectives of this work are the study of total energy of the phonon at temperature T , heat capacity of solids and Debye heat capacity model. The solid sample of metal such as (Al, Cu and Fe) of weight 0.25 Kg in an electric heater inserted completely inside a deep hole into the metal and a thermometer inside another deep hole. Both heater and thermometer must make good thermal contact with the sample. The metal was by an insulator. The theory of specific heat in solids shows that specific heat capacity for a material normally increases with temperature, due to the change in substance structure, more precisely, it depends on how many degrees of freedom are available in the substance particles, where a degree of freedom is a form of energy in which is stored in the object. Results show that, the average heat capacity of samples, at different temperatures from -90°C to 90°C are (Al=982.1140 j/mol. $^{\circ}\text{C}$, Cu =4740.3262 j/mol. $^{\circ}\text{C}$ and Fe =241.9965j/mol. $^{\circ}\text{C}$), take the uncertainties for the different measurements showed that accuracy depended very little on the sample. All though Debye heat capacity model is the best theoretical model to study the heat capacity in solids, modern research has revealed some

discrepancy in the model at low temperatures and that Debye's temperature is not a constant, but varies with temperature.

Keywords: Heat Capacity .Lattice Vibrations, Debye Model.

1. Introduction

There are two contributions properties of solid, one comes from phonons (or lattice vibrations) and another from electrons. This research is devoted to the thermal properties of solids due to lattice vibrations. Heat capacity is measurable physical quantity that characterizes the ability of a body to store heat as it changes in temperature. Consider simple solid containing N atoms. Now, atoms in solids cannot translate (unlike those in gases), but are free to vibrate about their equilibrium positions. Such vibrations are called lattice vibrations, and can be thought of as sound waves propagating through the crystal lattice. Each atom is specified by three independent position coordinates, and three conjugate momenta coordinate. Let us only consider small amplitude vibrations. In this case, we can expand the potential energy of interaction between the atoms to give an expression which

is quadratic in the atomic displacements from their equilibrium positions. It is always possible to perform a normal mode analysis of the oscillations. In effect, we can find $3N$ independent modes of oscillation of the solid [1,2]. The Lattice vibrations in metals can be particularly difficult to treat by starting from the standpoint of force constants. A special way of looking at lattice vibrations in metals has been given. Some metals can apparently be described by a model in which the restoring forces between ions are either of the bond- stretching or axially symmetric bond-bending variety. I have listed some other methods for looking at the vibration problems in Einstein model and Debye model [3, 4,5].

2. Material and Method

Experience tells us that if a sample of metal is added to electric heater, the temperature of the metal will rise. If several different metals having the same mass are heated to the same temperature. The ability of any material to retain heat energy is called that material's heat capacity. The measure of heat capacity, or the quantity of heat needed to raise the temperature of one gram of a substance by one degree Celsius, is termed specific heat and is represented by the symbol C_v .

3. Experiment Theory

$$C_v = \left(\frac{\partial E}{\partial T} \right)_v = \frac{12\pi^4}{5} Nk_B \left(\frac{T}{\theta_D} \right)^3 \quad (1)$$

Where N number of atoms, k_B Boltzmann constant, θ_D Debye temperature.

When we say we are differentiating at constant volume it may not be in the least evident where there could be any volume dependence. only in a crystal with a fixed volume, this effect is not relevant. This is not realistic as there is a thermal expansion of the solids. It would not be consistent to include anything about thermal expansion here. Thermal expansion is due to the harmonic terms in the potential and we are consistently neglecting these [6,7]. Furthermore, the Debye theory works fairly well in its present form

$$C_v = 402.4564 \times 10^{-23} \times N \left(\frac{T}{\theta_D} \right)^3 \quad (2)$$

The Figure (1) shows a simple form of laboratory apparatus. They used solid sample of metal such as (Al, Fe and Cu) 0.25 Kg with an electric heater element completely inside a deep hole bored into the metal and a thermometer inside another deep hole. Both Heater and Thermometer must make good thermal contact with the sample. An insulating jacket is placed round the metal.

The initial temperature is measured. Then the apparatus is heated for a time interval T at constant V and I . The final temperature is measured simultaneously with switching off the

electrical supply. The objectives of this experiment are measurements heat capacity of (*Al*), (*Cu*) and (*Fe*) at deferent temperature *T*.

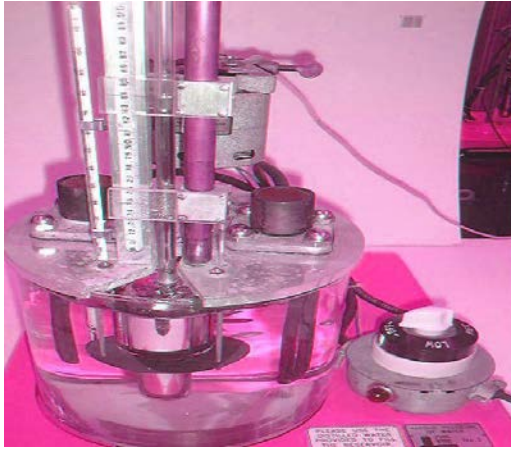


Fig (1): laboratory apparatus Measurement of Specific Heat Capacity

3. Tables and Figures

Table (1): heat capacity of (*Al*) at temperature from $-90^{\circ}C$ to $90^{\circ}C$.

$$N = 55.7974 \times 10^{23} \theta_D = 155^{\circ}C$$

No	T(°c)	T(°c)/θ _D	(T(°c)/θ _D) ³	C _v
1	-90	-0.58065	-0.019577	-3516.87233
2	-80	-0.51613	-0.13749	-2470.01184
3	-70	-0.54161	-0.15888	-1654.71496
4	-60	-0.38170	-0.05561	-1042.03625
5	-50	-0.32258	-0.03357	-603.03023
6	-40	-0.25806	-0.01719	-308.75148
7	-30	-0.19355	-0.00725	-130.25453
8	-20	-0.12903	-0.00215	-38.59394
9	-10	-0.06452	-2.68586	-4.82424
10	0	0	0	0

11	10	0.06452	2.68586	4.82424
12	20	0.12903	0.00215	38.59394
13	30	0.19355	0.00725	130.25453
14	40	0.25806	0.01719	308.75148
15	50	0.32258	0.03357	603.03023
16	60	0.38170	0.05561	1042.03625
17	70	0.54161	0.15888	1654.71496
18	80	0.51613	0.13749	2470.01184
19	90	0.58065	0.19577	3516.87233

Table (2): heat capacity of (*Cu*) at temperature from $-90^{\circ}C$ to $90^{\circ}C$.

$$N = 23.6914 \times 10^{23} \theta_D = 70^{\circ}C$$

No	T(°c)	T(°c)/θ _D	(T(°c)/θ _D) ³	C _v
1	-90	-1.28571	-2.12534	-16211.91582
2	-80	-1.14286	-1.49272	-11386.14664
3	-70	-1	-1	-7627.82870
4	-60	-0.85714	-0.62973	-4803.53061
5	-50	-0.32258	-0.36444	-2779.82096
6	-40	-0.57143	-0.18659	-1423.26833
7	-30	-0.42857	-0.07872	-600.44133
8	-20	-0.28571	-0.02332	-177.90854
9	-10	-0.14286	-0.00292	-22.23857
10	0	0	0	0
11	10	0.14286	0.00292	22.23857
12	20	0.28571	0.02332	177.90854
13	30	0.42857	0.07872	600.44133
14	40	0.57143	0.18659	1423.26833
15	50	0.71429	0.36444	2779.82096
16	60	0.85714	0.62973	4803.53061
17	70	1	1	7627.82870

18	80	1.14286	1.49272	11386.14664
19	90	1.28571	2.12534	16211.91582

Table (3): heat capacity of (Fe)at temperature from $-90^{\circ}C$ to $90^{\circ}C$.

$$N = 26.9585 \times 10^{23} \theta_D = 197^{\circ}C$$

No	T(°c)	T(°c)/θ _D	(T(°c)/θ _D) ³	C _V
1	-90	- 0.45685	- 0.09535	- 827.62725
2	-80	- 0.40609	- 0.06697	- 581.26907
3	-70	- 0.35533	- 0.04486	- 389.40486
4	-60	- 0.30457	- 0.02825	- 245.22289
5	-50	- 0.25381	- 0.01635	- 141.91139
6	-40	- 0.20305	- 0.00837	- 72.65863
7	-30	- 0.15228	- 0.00353	- 30.65286
8	-20	- 0.10152	- 0.00105	- 9.08233
9	-10	- 0.05076	- 1.30787	- 1.13529
10	0	0	0	0
11	10	0.05076	1.30787	1.13529
12	20	0.10152	0.00105	9.08233
13	30	0.15228	0.00353	30.65286
14	40	0.20305	0.00837	72.65863
15	50	0.25381	0.01635	141.91139
16	60	0.30457	0.02825	245.22289
17	70	0.35533	0.04486	389.40486

18	80	0.40609	0.06697	581.26907
19	90	0.45685	0.09535	827.62725

Fig (2): Heat capacities of samples (Al – black; Cu –

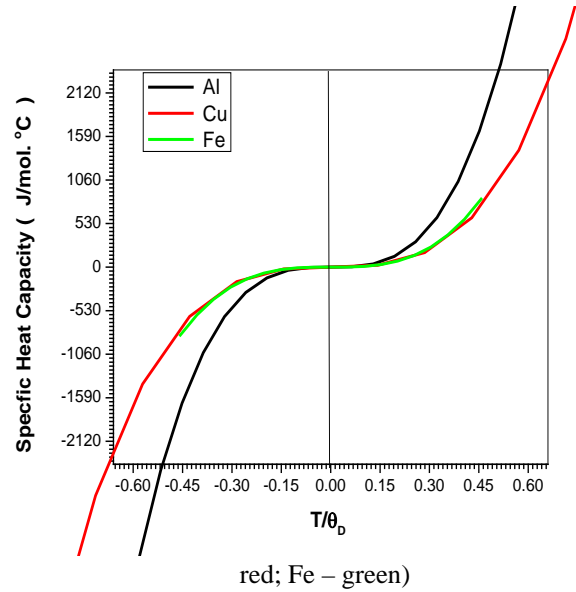
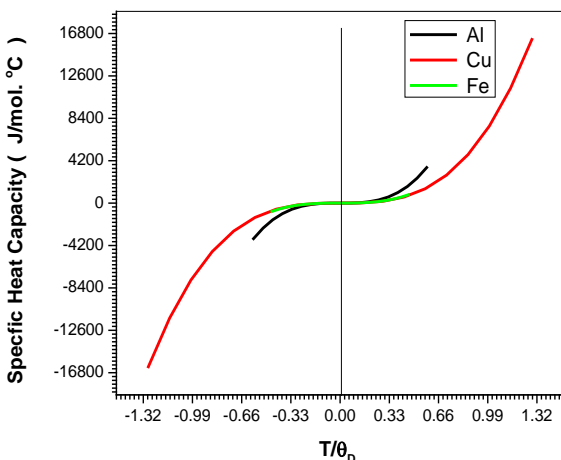


Fig (3): Heat capacities of samples (Al – black; Cu – red; Fe – green), transition part between $-0.6 \frac{T}{\theta_D}$ and $0.6 \frac{T}{\theta_D}$

4. Discussion

The theory of specific heat in solids shows that specific heat capacity for a material normally increases with increasing temperature, due to the specific heat capacity being a function of its own substance structure. More precisely, it depends on how many degrees of freedom available in the substance particles, where a degree of freedom is any form of energy in which heat transferred into an object can be stored. Debye heat capacity model is nowadays the best theoretical model for heat capacity in solids. Even though newer research



has revealed some discrepancy in the model at low temperatures and that Debye's temperature is not a constant, but varies with temperature. From Figure (4), it can be seen that the heat capacities of the samples increase with increasing temperature in a smooth and continuous manner in the experimental temperature range, in accordance with the theory of specific heat of solids in equation (2). Some of the curves increase in a smooth and continuous manner in the experimental range, while the sample of the samples curves in figure (3) has an abnormal transition part between $-0.6\frac{T}{\theta_D}$ and $0.6\frac{T}{\theta_D}$. This anomaly has so far not been possible to provide a background for. It has on the other hand been possible to rule out some of the possibilities causing this deviation in the curves.

5. Conclusions

In this work, the specific heat capacity for Al, Cu and Fe, have been measured using an Equation (2) method on differential scanning calorimeter from -90°C to 90°C . The average heat capacity of samples, at different temperatures from -90°C to 90°C are (Al=982.1140 $\text{j/mol.}^{\circ}\text{C}$, Cu =4740.3262 $\text{j/mol.}^{\circ}\text{C}$ and Fe =241.9965 $\text{j/mol.}^{\circ}\text{C}$). The inactivated sample

curves showed a general trend, where the heat capacities for inactivated material normally were higher than the heat capacities for the respective sample material. This presumption was stated mainly because the heat capacities for the inactivated samples increased in a smooth and continuous manner with increasing temperature, without this sudden heat capacity change around $-0.6\frac{T}{\theta_D}$. The conclusion is due to the time perspective of this work an assumption based on observations and personal experience.

6. References

- [1] Charles K, 2005 "Introduction to solid state physics". —8th ed. p. cm. ISBN 0-471-41526-X. Unite State of America.pp703.
- [2] Alexander A and Ben S, 2001"Concepts of Theoretical Solid State Physics¹" Unite State of America.pp703.
- [3] James D.P and Bernard C.B, 2006 "Solid-State Physics Introduction to the Theory" ISBN-10 3-540-24115-9 Berlin Heidelberg New York.pp727.
- [4] Bernhard K,(Ed.) 2006 "Advances in Solid State Physics"CampusRing1. 28757Bremen.Germany.b.kramer@iu-bremen.de.pp421.



[5] Charles K. 1987 "Quantum Theory of Solids" (John Wiley and Sons, New York).pp607.

[6] James D.P and Bernard C.B, 2006 "Solid-State Physics Introduction to the Theory" ISBN-10 3-540-24115-9 Berlin Heidelberg New York.pp727.

[7] Jiang C.H 2010 "Thermodynamic properties and heat capacities"(BTC) $\frac{1}{3}$ (DMF) (HCOO). Journal of Thermal Analysis and Calorimeters, 102(3): p. 1087-1093.