

University of Anbar  
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# فيزياء الحالة الصلبة Solid state Physics

المرحلة الرابعة  
الكورس الاول  
صلبة 1

## 7. Thermal properties

Thermal property *الخاصية الحرارية* refers *تشير الى* to the response *استجابة* of a material to the application *تطبيق* of heat *حرارة*. As a solid absorbs *تمتص* energy in the form *بشكل* of heat, its temperature rises *تزداد حرارتها*, and its dimensions *ابعادها* increase *تزداد*. The energy may be transported *تنتقل* to cooler regions *الاجزاء الباردة* of the specimen *العينة* if *اذا* temperature gradients exist *موجود*, and ultimately *وبانهاية*, the specimen may melt *ربما تذوب*. Heat capacity *السعة الحرارية*, thermal expansion *التمدد الحراري*, and thermal conductivity *التوصيلية الحرارية* are properties *الخصائص* of materials.

### 7.1 Specific Heat:

The specific heat per mole is defined as

$$C = \frac{\Delta Q}{\Delta T} \quad 7.1$$

where  $\Delta Q$  is the heat required *المطلوبة* to raise *لزيادة* the temperature of one mole by an amount equal *بكمية مساوية* to  $\Delta T$ . If the process *اذا العملية* is carried out *تمت* at constant volume *لحجم ثابت*, then  $\Delta Q = \Delta E$ , where  $\Delta E$  is the increase *الزيادة* in the internal energy *الطاقة الداخلية* of the system. The specific heat at constant volume  $C_v$ , is therefore given by

$$C_v = \left( \frac{\partial E}{\partial T} \right)_v \quad 7.2$$

The specific heat depends *تعتمد* on the temperature in the manner *بطريقة* shown in Fig. 7.1. At high temperatures the value of  $C_v$  is close to *قريبة من*  $3R$ , where  $R$  is the universal gas constant *ثابت الغازات العام*.

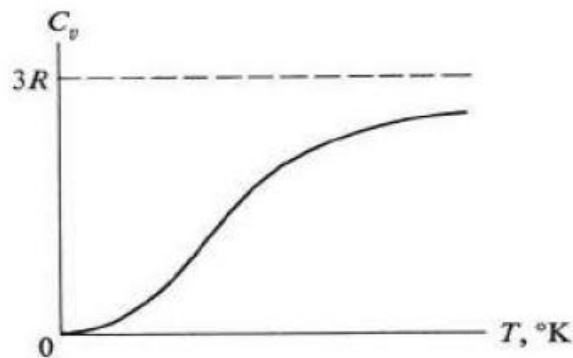


Figure 7.1 Dependence *اعتماد* of specific heat of solids on temperature.

The classical theory النظرية الكلاسيكية: The model used يستخدم to describe لوصف the solid is one in which كل ذرة is bound ترتبط to its site الى موقعها by a harmonic force بقوة توافقية. When the solid is heated تسخن, the atoms vibrate تهتز around their sites حول موقعها like مثل a set مجموعة of harmonic oscillators متذبذبات توافقية. The energy associated الطاقة المرافقة with this motion مع هذه الحركة is the energy E, from physics that the average energy معدل الطاقة  $\bar{\epsilon}$  for a one-dimensional oscillator لمتذبذب في بعد واحد is equal to  $kT$ , where  $k$  is the Boltzmann constant ثابت بولتزمان. That is,

$$\bar{\epsilon} = kT \quad 7.3$$

The average energy per atom, regarded اعتبر as a three-dimensional oscillator كمتذبذب ثلاثي الابعاد, is  $3kT$  and consequently the energy per mole is

$$E = 3N_A kT = 3RT \quad 7.4$$

where  $N_A$  is Avogadro's number. We have used the relation  $R = N_A k$

From equations 7.2 and 7.4 we find that

$$C_v = 3R \quad 7.5$$

This result هذه النتيجة is certainly من المؤكد in agreement مع تتوافق with experiment التجريبي at high temperatures, but it fails تفشل completely كلياً at low temperature.

This discrepancy تناقض between theory النظري and experiment التجريبي was one of the outstanding مفارقات paradoxes بارزة in physics until 1905, when it was resolved تم حلها by Einstein العالم انيشتاين, when he used عندما استخدم the new quantum mechanics الميكانيك الكمي الحديث.

### 7.1.1 The Einstein model:

In this model في هذا الموديل, the atoms فان الذرات are treated تعامل as independent oscillators لمتذبذب, but لكن the energy الطاقة of the oscillator is given تعطى by quantum mechanics بالميكانيك الكمي rather than by the classical الكلاسيكي, the result according النتيجة تبعاً to quantum mechanics, the energy of an isolated oscillator لمتذبذب معزول is restricted محدد to the values القيم

$$\epsilon_n = n\hbar\omega \quad 7.6$$

where  $n$  is a positive integer or zero. That is,  $n = 0, 1, 2, \dots$ . The constant

$\omega$  is the frequency **التردد** of the oscillator **المتذبذب**. Thus, the energy of the oscillator is quantized **مكممة**.

The energy **الطاقة** of the oscillator is therefore **لذلك تكون** continually changing **مستمرة التغير**, but its average value **معدل القيمة** at thermal equilibrium **التوازن الحراري** is given by,

$$\bar{\epsilon} = \frac{\sum_{n=0}^{\infty} \epsilon_n e^{-(\epsilon_n/kT)}}{\sum_{n=0}^{\infty} e^{-\epsilon_n/kT}} \quad 7.7$$

The exponential  $e^{-\epsilon_n/kT}$  is the well-known **Boltzmann factor** **معامل يعرف**, which gives **الاحتمالية** the probability **والذي يعطي** that the energy state  $\epsilon_n$  is occupied **محتمل او مشغول**, **حالة الطاقة**.

$$\bar{\epsilon} = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1} \quad 7.8$$

We can now **نستطيع الان** find **ايجاد** the energy of the solid by noting **بملاحظة** that each atom **ذرة** is equivalent **تكافئ** to three oscillators **ثلاث متذبذبات**, so that **لذلك** there is **يوجد** a total of  $3N_A$  such oscillators. The total energy is, therefore,

$$E = 3N_A \frac{\hbar\omega_E}{e^{\hbar\omega_E/kT} - 1} \quad 7.9$$

where we used  $\omega_E$ , the Einstein frequency **تردد انيشتاين**, to denote **لنرمز الى** the common frequency **التردد المشترك** of the oscillators **للمتذبذبات**. The specific heat, found by differentiating **باشتقاق** this expression as in equation 7.2 and  $R = N_A k$ ,

$$C_v = 3R \left( \frac{\hbar\omega_E}{kT} \right)^2 \frac{e^{\hbar\omega_E/kT}}{(e^{\hbar\omega_E/kT} - 1)^2} \quad 7.10$$

This equation **هذه المعادلة** may be simplified **يمكن ان تبسط** by introducing **بتقديم**, the **Einstein temperature**  $\theta_E$  **حرارة انيشتاين**

where  $k\theta_E = \hbar\omega_E$ . therefore,  $\theta_E = \hbar\omega_E/k$

Expression above then reduces to

$$C_v = 3R \left( \frac{\theta_E}{T} \right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2} \quad 7.11$$

In low temperature range, in which  $T \ll \theta_E$

$$c_V = 3R \left( \frac{\theta_E}{T} \right)^2 e^{-\theta_E/T} \quad 7.12$$

**At high Temperature Limit  $T \gg \theta_E$**

In the high-temperature limit, where  $T \gg \theta_E$ , one may expand the exponential  $e^{\theta_E/T}$  in a power series of  $\theta_E/T$ . Carrying this out and retaining only the largest terms in the series, one finds that  $C = 3R$ , which is the classical result

$$e^{\theta_E/T} = 1 + \frac{\theta_E}{T} \quad \therefore \quad c_V = 3R \quad 7.13$$

This result is in agreement المحصل عليها مع النتيجة with the result تنفق obtained by classical theory النظرية الكلاسيكية at high temperature في درجات الحرارة العالية.

### 7.1.2 The Debye model:

The atoms in the Einstein model were assumed to oscillate independently of each other. Actually, the idea of independence here is not a viable one because, since the atoms do interact with each other, the motion of one atom affects its neighbors. The motion of these in turn affects their neighbors, and so forth, so that the motion of one atom anywhere in the solid, in fact, affects all other atoms present. Thus, we need to consider the motion of the lattice as a whole, and not a single independent atom. That is, we must consider the collective lattice modes.

The most familiar example of such collective modes is the sound waves in solids. When a sound wave propagates in a solid, the atoms do not oscillate independently; their motions are orchestrated in such a manner that they all move with the same amplitude and with a fixed phase relationship.

Debye assumed افترض ديبي that all these modes have a character similar خاصية تشبه to sound waves موجات الصوت.

Now let us calculate specific heat on the basis of the Debye model. In finding the energy of vibration, we note that each mode is equivalent to a single harmonic oscillator. The total energy of vibration for the entire lattice is now given by the expression

$$E = \int \bar{\epsilon}(\omega) g(\omega) d\omega, \quad 7.14$$

Here  $g(\omega)$  is the density-of-states function, follows from noting that  $g(\omega) d\omega$  is the number of modes in the range  $(\omega, \omega + d\omega)$ , and the energy of each of these modes is equal to  $\bar{\epsilon}(\omega)$ , The ensuing expression for the total energy is

$$E = \frac{3V}{2\pi^2 v_s^3} \int \omega^2 \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1} d\omega \quad 7.15$$

Before we can evaluate the integral, we need to know its limits, namely, the lower and upper ends of the frequency spectrum. The lower limit is evidently  $\omega = 0$ . The upper cut off frequency was determined by Debye, by requiring that the total number of modes included must be equal to the number of degrees of freedom for the entire solid. Since this number is equal to  $3N_A$ , because each atom has three degrees of freedom, the above condition may be expressed in terms of the density of states as

$$\int_0^{\omega_D} g(\omega) d\omega = 3N_A \quad 7.16$$

where the cutoff frequency **تردد القطع**, denoted **يرمز ل** by  $\omega_D$ , is called the **Debye frequency** **تردد ديبي**.

The Debye frequency can be determined by substituting for  $g(\omega)$

$$\omega_D = v_s (6\pi^2 n)^{1/3} \quad 7.17$$

where  $n = N_A/V$ , is the concentration of atoms in the solid,  
the total energy is now given by

$$E = \frac{3V}{2\pi^2 v_s^3} \int_0^{\omega_D} \frac{\hbar \omega^3}{e^{\hbar \omega / kT} - 1} d\omega \quad 7.18$$

the specific heat  $C_v$ , which is found by differentiating this equation with respect to  $T$ , is

$$C_v = \frac{3V}{2\pi^2 v_s^3} \frac{\hbar^2}{k T^2} \int_0^{\omega_D} \frac{\omega^4 e^{\hbar \omega / kT}}{(e^{\hbar \omega / kT} - 1)^2} d\omega \quad 7.19$$

We can simplify the appearance of this equation by changing to a dimensionless variable  $x = \hbar \omega / kT$ , and by defining the **Debye temperature**  $\theta_D$  as  $k\theta_D = \hbar \omega_D$ .

$$C_v = 9R \left( \frac{T}{\theta_D} \right)^3 \int_0^{\theta_D / T} \frac{x^4 e^x}{(e^x - 1)^2} dx \quad 7.20$$

When  $\theta_D \ll T$ , so  $x$  is small &  $e^x = 1 + x + \frac{x^2}{2} + \dots$

so the upper limit of the integral is very small, In the first approximation, the integral reduces to

$$\int_0^{\theta_D / T} x^2 dx = \frac{1}{3} (\theta_D / T)^3$$

which leads to

$$C_v = 3R$$

When  $T \ll \theta_D$  and hence the upper limit of the integral approaches  $\infty$ . The ensuing integral

$$\int_0^{\infty} [x^4 / (e^x - 1)^2] dx$$

The specific heat is now given by

$$C_v = \frac{12\pi^4}{5} R (T / \theta_D)^3 \quad 7.21$$

## 7.2 Thermal conductivity

When the two ends of a sample of a given material are at two different temperatures,  $T_1$ , and  $T_2$  where ( $T_2 > T_1$ ), heat flows down the thermal gradient, from the hotter to the cooler end, as shown in figure below.

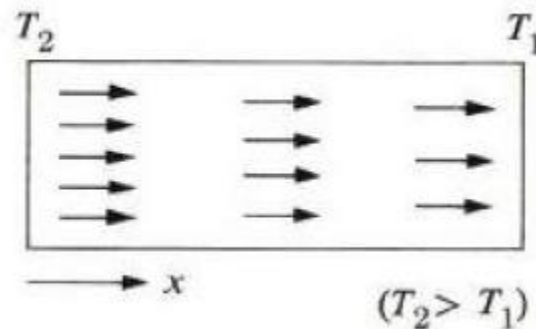


Figure 7.2 Thermal conduction by lattice waves

The heat current density  $Q$  (the current per unit area) is proportional to the temperature gradient ( $\partial T / \partial x$ ).

$$Q = -K \frac{\partial T}{\partial x}$$

7.22

The proportionality constant  $K$ , known as the **thermal conductivity**.

Heat may be transmitted in the material by several independent agents. In metals, for example, the heat is carried both by electrons and by lattice waves, or phonons, although the contribution of the electrons is much the larger.

In insulators, on the other hand, heat is transmitted entirely by phonons, since there are no mobile electrons in these substances.

In particular, thermal conductivity is given by

$$K = \frac{1}{3} C_v v l$$

7.23

where  $C_v$ , is the specific heat per unit volume,  $v$  the speed of the particle, and  $l$  its mean free path.



### 7.3 Thermal Expansion التمدد الحراري

Most **معظم** solid materials expand **تتمدد** upon heating **بالحرارة** and contract **وتتقلص** when cooled **بالبرودة**. The change **التغير** in length **بالطول** with temperature for a solid material may be expressed as follows:

$$\frac{l_f - l_0}{l_0} = \alpha_l (T_f - T_0) \quad \text{or} \quad \frac{\Delta l}{l_0} = \alpha_l \Delta T$$

where  $l_0$  and  $l_f$  represent, respectively, initial **بدائي** and final **نهائي** lengths with the temperature change **تغير درجة الحرارة** from  $T_0$  to  $T_f$ . The parameter  $\alpha_l$  is called the **linear coefficient of thermal expansion** **المعامل الخطي للتمدد الحراري**; it is a material property **خاصية** that is indicative **تدل على** of the extent **مدى** to which a material expands **تتوسع** upon heating **بالتسخين** and has units **ولها وحدات** of reciprocal temperature  $^{\circ}\text{C}^{-1}$ .

heating or cooling affects **تؤثر** all the dimensions **جميع ابعاد** of a body, with **مع** a resultant change **تغير ناتج** in volume **في الحجم**. Volume changes **تغيرات الحجم** with temperature may be computed **تحسب** from

$$\frac{\Delta V}{V_0} = \alpha_v \Delta T$$

where  $\Delta V$  and  $V_0$  are the volume change **التغير بالحجم** and the original volume **الحجم**, respectively **على التتابع**, **الاصلي**. And  $\alpha_v$  symbolizes **يرمز الى** **المعامل الحجمي للتمدد الحراري**.

#### References المصادر المعتمدة في هذا الكورس

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- 3- M. A. OMAR Elementary-solid-state-physics