

# Thermodynamic Properties, Mechanical Properties and Interatomic Potential in Solids. A *Shou-Shi-Ling* (手勢令) Game

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## Abstract

Two formulae were developed to express sublimation enthalpy and Young's modulus on a thermodynamic basis. The first formula reveals how the sublimation enthalpy is correlated with the thermal expansion coefficient and heat capacity of solids, whereas the second formula relates the Young's modulus with sublimation enthalpy and equilibrium interatomic (intermolecular) distance. These two formulae provide alternative ways to quantitatively estimate thermodynamic or mechanical properties of great importance in the development of new materials.

**Keywords:** Thermal Expansion Coefficient ; Heat Capacity ; Sublimation Enthalpy ; Young's Modulus

## 1 Introduction

We are living in a time when new materials have been designed and developed at an extraordinary speed to serve various purposes in scientific research and industrial practices. No matter it is a pharmaceutical or food related compound, or a solid pollutant: sublimation enthalpy has long been recognized as one of the most important thermodynamic parameters in the estimation of the solubility and the volatilization ability under various conditions [1-9]. Up to date, there are usually four direct methods, namely the mass effusion Knudson (ME), the quartz crystal microbalance (QCM), the transpiration method and thermogravimetric analysis (TGA), used to determine the sublimation enthalpy [10]. Although all these four direct methods are applicable to the low volatile compounds and even tolerate the impurity, especially the TGA method, with all these methods, the accuracy of the results demands highly operator experience and are limited to the sublimation enthalpy at 298 K. To overcome these limitations, some indirect yet quite effective methods have been proposed [11-14]. Others employed a computational strategy to derive the value of sublimation enthalpy. A group contribution (GC) method based on the statistical analysis was used to predict the sublimation enthalpy of organic compounds with cyclic structure [15]. However, the applicability of such a methodology is restricted organic compounds with cyclic structure. Semi-empirical models have been recently developed in order to provide theoretical strategies for the prediction of the sublimation enthalpy of organic contaminants from their 3D molecular structure, by integrating gene expression programming (GEP) and quantitative structure–property relationship (QSPR) modelling. [16] Other empirical relationships involving sublimation enthalpy and other

thermodynamical quantities of organic crystals were recently proposed by Chickos and Gavazzotti [17]. In their colossal work, the Authors present a database consisting of 1655 critically evaluated sublimation enthalpies of organic compounds, along with a solid statistical analysis; an important conclusion was that the intrinsic accuracies of calculated lattice energies and experimental sublimation enthalpies are similar ( $\sim 5\text{--}10\text{ kJ mol}^{-1}$ ). On the other hand, quantum mechanical methods were also employed to estimate the value of the sublimation enthalpy [18]. Besides the potential expense bounded with the large request of memory and machine time and the complication due to the performance of different functionals and basis sets depending on the investigated system, the results obtained through quantum mechanical calculation exhibited significant deviation from the experimental results.

For the characterisation of some new materials, their mechanical properties also become extremely important. A representative of such new materials, lithium ion conductor, has been used as the solid state electrolyte in lithium battery. With their various composite and crystalline features, lithium ion conductors have attracted extensive attention because of their chemical/physical stability and high conductivity and therefore, have been widely used in the portable electronics and finding their applications to the electric vehicles [19-22]. Young's modulus is an important parameter to characterise the solid state electrolytes, as the elastic property plays a key role in the determination of the overall performance of the solid state electrolyte [23]. However, the measured mechanical properties for the lithium ion conductors have been scarce. The Young's modulus may be obtained through

direct measurement using either acoustic impulse excitation or nanoindentation [24-26], alternatively, or through quantum mechanical calculation [19, 27].

On the other hand, the thermostability of the solid state electrolytes directly affects its conductivity and the overall performance in the lithium battery [28]. Other than heat capacity, the thermal expansion coefficient is very important thermodynamic parameter for lithium ion conductor, especially when the conductivity needs to be optimized through doping and annealing process [29]. Sometimes, the thermal expansion coefficient of the solid state electrolyte is a good reference to evaluate the performance and durability of lithium battery at the operating temperature [30].

It is noticed that such mechanical and thermal properties that seem to be quite critical in the characterization of the solid state electrolytes are equally important for other materials such as alloys, super conducting materials, as well as plastics and cements. For instance, the thermal expansion of a 2D supramolecular assembly of polyphenylene was studied using the combination of high resolution atomic force microscopy and dynamic simulation at different temperatures, and the non-covalent intermolecular interaction was believed to take responsibility of the huge thermal expansion coefficient obtained for such supramolecular assembly [31]. No matter it is a sublimating process or an elastic testing: any mechanical and thermodynamical property depends on the type of interactions existing between the atoms, ions, or molecules constituting that material. These interactions are conveniently expressed in a mathematical form reflecting the potential energy function. In this work, we developed a simple analytical model to express relationships among three key elements in the study of the matter structure: thermodynamic properties, mechanical properties and the

interatomic potential (including structural information). We shall show how these quantities are bounded each other, and dependently on the context, and one can be readily derived if the others are known, by playing this simple, yet effective “*Ro Sham Bo!*” game.<sup>1</sup> More importantly, the present model provides a theoretical foundation to the empirical and semi-empirical relationships so far presented in the Literature and hence may be used to accurately estimate the value of sublimation enthalpy even with the low volatile compounds, and the value of Young’s modulus simply using the measured thermal expansion coefficient, specific heat capacity, thermal expansion coefficient and the intermolecular/nuclear distance obtained from X-Ray diffraction spectroscopy. Such practice should be beneficial to both scientific research and industrial practice.

## 2 Model

An interaction potential expresses the mathematical connection between the energy of the system and its structure. For bounded systems, they show one or more minima, corresponding to a certain geometrical arrangement, which is said equilibrium geometry,  $r_e$ . As underlined in a recent work [32], for anharmonic (non-symmetric) potentials this value does not correspond to the geometry of the system, even when the zeroth vibrational level is populated, due to a non-null shift called “zero point position”, ZPP. Dependently of the type of system and the targets of the investigation, the best choice for the most convenient

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<sup>1</sup> According to Moore and Sward, the first known mention of this game was contained in the book *Wuzazu* by the Chinese Ming-dynasty writer Xie Zhaozhi; he wrote that the game – called *shoushiling* – had origin back to the time of the Han dynasty (206 BC – 220 AD). The game is also mentioned in the book *Note of Liuyanzhai* by Li Rihua. See Moore, M. E.; Sward, J. “Introduction to the game industry” (2006) Upper Saddle River, NJ: Pearson Prentice Hall. p. 535.

analytical, yet empirical expression of the interaction potential may change. In particular, we may distinguish the case of ionic solids from that of metallic or molecular solids. For the former, a widely used expression for the potential is the Born-Mayer potential:[33]

$$\Phi(r) = -\frac{\mathcal{M}}{4\pi\epsilon_0} \frac{z_+ z_- e^2}{r} + \frac{B}{r^n}, \quad (1)$$

where  $\mathcal{M}$  indicates the Madelung constant, and  $B$  can be obtained from the equilibrium condition,  $\frac{d\Phi}{dr} = 0$ :

$$B = \frac{\mathcal{M}}{4\pi\epsilon_0} \frac{z_+ z_- e^2}{n} r_e^{n-1}. \quad (2)$$

In the case of metallic or molecular solids, among the many, here we remind the Morse potential:[34]

$$\Phi(r) = D_e \left[ 1 - e^{-a(r-r_e)} \right]^2, \quad (3)$$

and the Lennard-Jones (L-J) potential that in a general form reads:[35]

$$\Phi(r) = D_e \left\{ 1 + \frac{mn}{n-m} \left[ -\frac{r_e/r^m}{m} + \frac{r_e/r^n}{n} \right] \right\}, \quad (4)$$

where  $D_e$  indicates the dissociation energy (from the bottom of the well). The value of this parameter may be conveniently estimated from spectroscopical or thermodynamical measurements, and in particular from the experimental molar sublimation enthalpy,  $\Delta H_{subl}$ :

$$D_e = \frac{2\Delta H_{subl}}{N\nu}. \quad (5)$$

where  $\nu$  indicates the coordination number and  $N$  the Avogadro constant. The two numerical parameters  $m, n$  appearing in eq (4) are usually constrained to specific, integer values (*viz.*,  $m = 6$  and  $n = 12$ ); Lennard-Jones [36] found this simplification successful in the theory of the virial coefficient of gases and used it also in his order-disorder theory of melting. In this work, we decided for a more general and flexible expression of the potential. Upon the introduction of the elongation,  $\Delta r \equiv r - r_e$ , the L-J potential (4) may be re-written as:

$$\Phi(\Delta r) = D_e \left\{ 1 + \frac{mn}{n-m} \left[ -\frac{1}{m} \left( \frac{1}{1 + \Delta r / r_e} \right)^m + \frac{1}{n} \left( \frac{1}{1 + \Delta r / r_e} \right)^n \right] \right\}. \quad (6)$$

If  $\Delta r / r_e \ll 1$ , eq (6) can be expanded in series, by reminding that:

$$1 - x^{-p} = 1 - px + \frac{p(p+1)}{2!} x^2 - \frac{p(p+1)(p+2)}{3!} x^3 + \dots, \quad (7)$$

and hence:

$$\begin{aligned} \Phi(\Delta r) &= D_e \left\{ \frac{mn}{2} \left( \frac{\Delta r}{r_e} \right)^2 - \frac{mn(m+n+3)}{6} \left( \frac{\Delta r}{r_e} \right)^3 + \right. \\ &\quad \left. + \frac{mn[m^2 + m(n+6) + n+11]}{24r_e^4} \left( \frac{\Delta r}{r_e} \right)^4 + \dots \right\}, \\ &= a(\Delta r)^2 + b(\Delta r)^3 + c(\Delta r)^4 + \dots \end{aligned} \quad (8)$$

where:

$$a \equiv \frac{mn}{2r_e^2} D_e, \quad (9)$$

$$b \equiv -\frac{mn}{6r_e^3} \frac{m+n+3}{D_e}, \quad (10)$$

$$c \equiv \frac{mn}{24r_e^4} \left[ m^2 + \frac{m+n}{n+6} + 11 \right] D_e. \quad (11)$$

The meaning of  $a$  is evidently bounded with the fundamental frequency  $\omega_0$  of vibration of one particle about the equilibrium position, *viz.*  $\omega_0 = \sqrt{a/\mu}$ , being  $\mu$  the reduced mass of the system. If we truncate the expansion (8) up to the forth power,

$$\Phi(x) \cong \alpha x^2 - \beta x^3 + \gamma x^4, \quad (12)$$

with  $x \equiv \Delta r$ , the Boltzmann factor can approximate:

$$e^{-\frac{\Phi(x)}{k_B T}} \cong e^{-\frac{\alpha x^2 - \beta x^3 + \gamma x^4}{k_B T}} = e^{-\frac{\alpha x^2}{k_B T}} e^{\frac{\beta x^3 + \gamma x^4}{k_B T}} \cong e^{-\frac{\alpha x^2}{k_B T}} \left( 1 + \frac{\beta x^3 + \gamma x^4}{k_B T} \right), \quad (13)$$

Classically, the average elongation can be calculated as:

$$\langle x \rangle \cong \frac{\int_{-\infty}^{+\infty} dx x e^{-\frac{\Phi(x)}{k_B T}}}{\int_{-\infty}^{+\infty} dx e^{-\frac{\Phi(x)}{k_B T}}} = \frac{\frac{3\sqrt{\pi}}{4} \frac{\beta}{[\alpha / k_B T]^{5/2}}}{\frac{\sqrt{\pi}}{4\alpha} \frac{4\alpha^2 + 3\gamma k_B T}{[\alpha / k_B T]^{3/2}}} = \frac{\beta}{\frac{4}{3} \frac{\alpha^2}{k_B T} + \gamma}, \quad (14)$$



and hence:

$$\langle \Delta r \rangle \cong \frac{-b}{\frac{4}{3} \frac{a^2}{k_B T} - c}. \quad (15)$$

We may further simplify this expression if the anharmonicity is not particularly strong, and only the first term may be accounted for ( $c \cong 0$ ):

$$\langle \Delta r \rangle \cong -\frac{3}{4} \frac{b}{a^2} k_B T. \quad (16)$$

In the limit of high temperatures:

$$\langle \Delta r \rangle \cong -\frac{3}{4} \frac{b}{a^2} \langle \varepsilon \rangle = -\frac{3}{4} \frac{b}{a^2} \frac{E}{3N}, \quad (17)$$

hence:

$$\frac{\langle \Delta r \rangle}{r_e} \cong \frac{m+n+3}{6mn} \frac{E/N}{D_e}. \quad (18)$$

We can also approximate  $E \cong H$  and plug (5) into (18), so to get:

$$\frac{\langle \Delta r \rangle}{r_e} \cong \nu \frac{m+n+3}{12mn} \frac{H}{\Delta H_{subl}}. \quad (19)$$

Since the heat capacity  $C_p \equiv \left( \frac{\partial H}{\partial T} \right)_p$ , by differentiating eq (19) with respect to temperature

at constant pressure, we obtain:

$$\left[ \frac{\partial}{\partial T} \left( \frac{\langle \Delta r \rangle}{r_e} \right) \right]_p = \left( \nu \frac{m+n+3}{12mn\Delta H_{subl}} \right) \left( \frac{\partial H}{\partial T} \right)_p = \Xi \frac{C_p}{\Delta H_{subl}}, \quad (20)$$

where  $\Xi \equiv \frac{\nu}{4mn} \left( \frac{m+n}{3} + 1 \right)$  contains information on the interatomic potential. This allows to put the thermal expansion coefficient,  $\lambda = \lambda(T)$ , in relationship with the sublimation enthalpy, the heat capacity, and the interatomic potential parameters, since:

$$\lambda \equiv \frac{1}{r_e} \frac{\partial r}{\partial T} = \frac{1}{r_e} \frac{\partial \langle \Delta r \rangle + r_e}{\partial T} = \frac{\partial}{\partial T} \left( \frac{\langle \Delta r \rangle}{r_e} \right) = \Xi \frac{C_p}{\Delta H_{subl}}. \quad (21)$$

This expression, which can be used only in the limit of high temperatures, provides a useful tool whence to estimate two among three parameters  $\alpha, \Delta H_{subl}, C_p$  being the other two known. In particular it reveals its usefulness for the evaluation of  $\Delta H_{subl}$ , since its direct measurement requires not negligible efforts and non-conventional equipment:

$$\Delta H_{subl} = \Xi \frac{C_p}{\lambda}. \quad (22)$$

Let consider now the connection with respect to the mechanical properties. The Young modulus,  $E$ , is defined as the ratio between stress,  $\sigma$ , and strain applied in the direction of the stress,  $\varepsilon_\sigma$ :

$$E \equiv \sigma / \varepsilon_\sigma. \quad (23)$$

where:

$$\sigma = q f_{\sigma}, \quad (24)$$

$$\varepsilon_{\sigma} = \Delta r / r_e, \quad (25)$$

where  $q$  indicates the number of atoms (or particles) per unit cross-sectional area, which can be approximated to  $q \cong \rho / M^{2/3}$ , being  $M = M_{\text{uma}} / N$ , and  $f_{\sigma}$  the force applied in the direction of the stress:

$$f_{\sigma} = f_{\text{eff}} = f \overline{\cos \theta}, \quad (26)$$

where:

$$f \equiv - \frac{\partial \Phi}{\partial r}, \quad (27)$$

$$\overline{\cos \theta} \equiv \frac{1}{\pi/2} \int_0^{\pi/2} \cos \theta d\theta = \frac{2}{\pi}, \quad (28)$$

being  $\theta$  the angle formed by the direction of application of the external force and the direction of the interatomic force. By differentiating the L-J potential (4), the force (27) reads:

$$\begin{aligned}
f_r &= D_e \frac{mn}{n-m} \frac{1}{r} \left[ r_e / r^m - r_e / r^n \right] \\
&= D_e \frac{mn}{n-m} \frac{1}{r_e} \left[ \left( \frac{1}{1 + \Delta r / r_e} \right)^{m+1} - \left( \frac{1}{1 + \Delta r / r_e} \right)^{n+1} \right] \\
&\cong D_e \frac{mn}{n-m} \frac{1}{r_e} \left\{ \left[ 1 - m + 1 \frac{\Delta r}{r_e} \right] - \left[ 1 - n + 1 \frac{\Delta r}{r_e} \right] \right\}, \\
&= mn \frac{D_e}{r_e} \left( \frac{\Delta r}{r_e} \right)
\end{aligned} \tag{29}$$

and therefore:

$$f_\sigma \cong \frac{2}{\pi} mn \frac{D_e}{r_e} \left( \frac{\Delta r}{r_e} \right), \tag{30}$$

$$\sigma \cong q \frac{2}{\pi} mn \frac{D_e}{r_e} \left( \frac{\Delta r}{r_e} \right), \tag{31}$$

$$E \cong q \frac{2}{\pi} mn \frac{D_e}{r_e} \cong \frac{\rho / M^{2/3}}{N\pi} \frac{4mn}{\nu} \frac{\Delta H_{subl}}{r_e}. \tag{32}$$

Eq (32) shows a connection between a mechanical property (the Young modulus), a thermodynamic property (the sublimation enthalpy) and the parameters defining the interatomic potential. Combining eq (32) and eq (22) we get:

$$E \cong \frac{\rho / M^{2/3}}{N\pi} \left( \frac{m+n}{3} + 1 \right) \frac{C_p}{\lambda r_e}. \tag{33}$$

### 3 Verification of the Model

In order to verify the proposed simple model, we considered two types of systems, *viz.* some metals and organic compounds. There could be different possible ways to apply the described theory in order to get one quantity from the others. In our opinion, the usefulness of the proposed model is more evident when employed to estimate quantities that are hard to access experimentally. We therefore decided to compare the Literature data of sublimation enthalpy and Young modulus with the values provided by eqs (22) and (33), respectively. In order to avoid the introduction of too much variety into the model with a consequent “blurriness” of our intents, we restricted ourselves to the simplified 6-12 L-J potential; so the potential itself was not parameterised to fit experimental data. As for the equilibrium distances  $r_e$ , the used values were therefore those obtained from the fitting of the Morse potential on the experimental data. Although the potential function used in this work is different (LJ potential, eq (4)), we may reasonably assume that the minima of the two potential functions coincide.

Table 1 collects data for the selected metals, and Figure 1 depicts the comparison. In order to compute the values predicted by the model, we chose to use the values of the physical quantities as measured at the high temperature, when available. The values predicted by the model are in good agreement with the Literature data; for both the equations, the least-square regression procedure shows a good linearity (Adj.- $R^2 = 0.9968$  and  $0.9672$  for eq (22) and (23), respectively), small values of intercept ( $a_0 = 6.6$  kJ/mol and  $12.6$  GPa, respectively) and slope close to unit ( $a_1 = 0.9855$  and  $0.9730$ , respectively). In general, it seems that sublimation enthalpy is better described. As for the Young modulus, the most

problematic cases are represented by zinc and iron. The poor prediction in these cases might be attributed to the lack of parameterisation of the L-J potential.

**Table 1.** Experimental and Computed properties of selected metals.

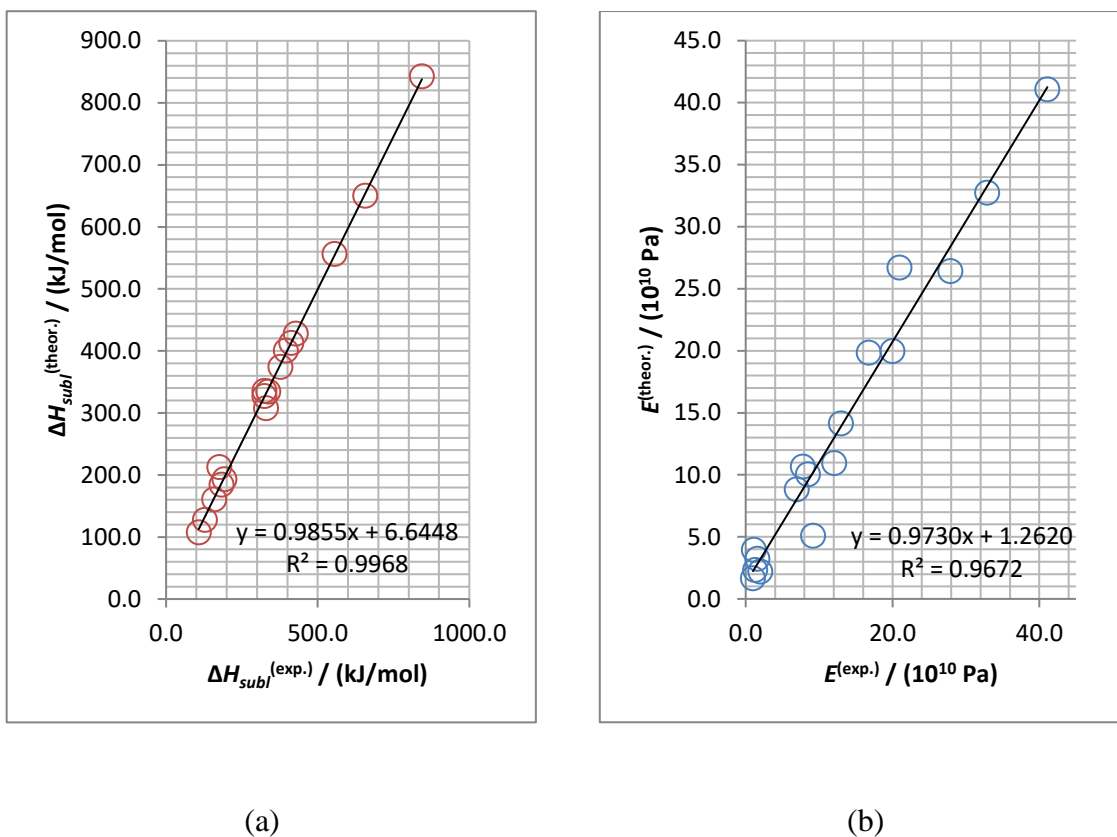
metal	$r_e / \text{\AA}$	$M / \text{uma}$	$\rho / (\text{g} \cdot \text{cm}^{-3})$	$\lambda / (10^{-6} \text{ K}^{-1})$	$C_p / (\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1})$	$\Delta H_{sub} / (\text{kJ} \cdot \text{mol}^{-1})$	$E / (10^{10} \text{ Pa})$	$\Delta H_{sub} / (\text{kJ} \cdot \text{mol}^{-1})$	$E / (10^{10} \text{ Pa})$
	*	**	**	***	**	****	**	eq (22)	eq (33)
Ag	3.11500	107.87	10.49	22.6	25.3	324.0	8.5	327.1	10.0
Al	3.40680	26.98	2.70	23.1	24.4	330.0	7.0	308.0	8.8
Au	3.02420	196.97	19.30	22.1	25.4	324.0	7.8	335.6	10.7
Ba	5.37300	137.33	3.51	25.7	28.2	176.0	1.3	213.0	2.3
Ca	4.56900	40.08	1.55	38.2	25.3	192.0	2.0	193.1	2.2
Cr	2.75400	52.00	7.19	11.3	23.3	395.4	27.9	400.8	26.4
Cu	2.89850	63.55	8.96	21.3	24.4	337.2	13.0	334.5	14.1
Fe	2.84500	55.85	7.87	11.8	25.1	413.0	21.0	413.2	26.7
Li	5.00160	6.94	0.54	30.0	24.8	159.0	1.2	160.6	3.9
Mo	3.04200	95.95	10.28	7.2	24.1	657.3	32.9	650.4	32.7
Na	5.36780	22.99	0.97	51.0	28.3	108.0	1.0	107.8	1.6
Ni	2.75837	58.69	8.91	17.8	26.1	428.0	20.0	428.0	20.0
Pb	3.73300	207.20	11.34	41.6	26.3	182.8	1.6	184.5	3.2
Pd	3.61631	106.42	12.02	19.9	25.5	376.8	12.1	374.3	10.9
Pt	2.91049	195.08	21.45	13.6	25.9	555.3	16.8	556.4	19.8
W	3.09200	183.84	19.25	5.6	24.3	843.5	41.1	842.6	41.1
Zn	2.59300	65.38	7.14	57.9	25.4	128.5	9.2	127.8	5.1

\* from [32]

\*\* from [37]

\*\*\* from [38]

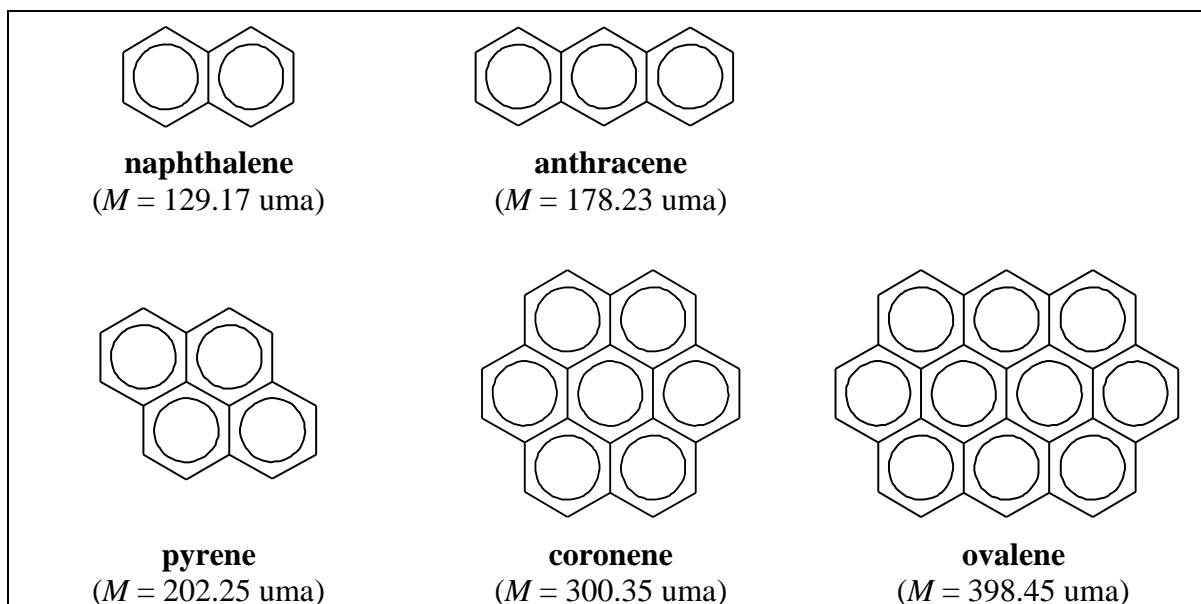
\*\*\*\* from [39]



**Figure 1.** Comparison between predicted and experimental values of (a) sublimation enthalpies and (b) Young modulus for the selected metals. The linear regression is also depicted.

The model was also tested on organic molecules. In the case of organic systems the choice is limited due to the scarcity of needed data. Only five polycyclic aromatic hydrocarbons (PAHs) were therefore considered, *viz.* naphthalene, anthracene, pyrene, coronene and ovalene (Chart 1). Table 2 collects numerical data for the selected PAHs, and Figure 2 depicts the comparison. Also for these systems it seems that the correlation is rather good.





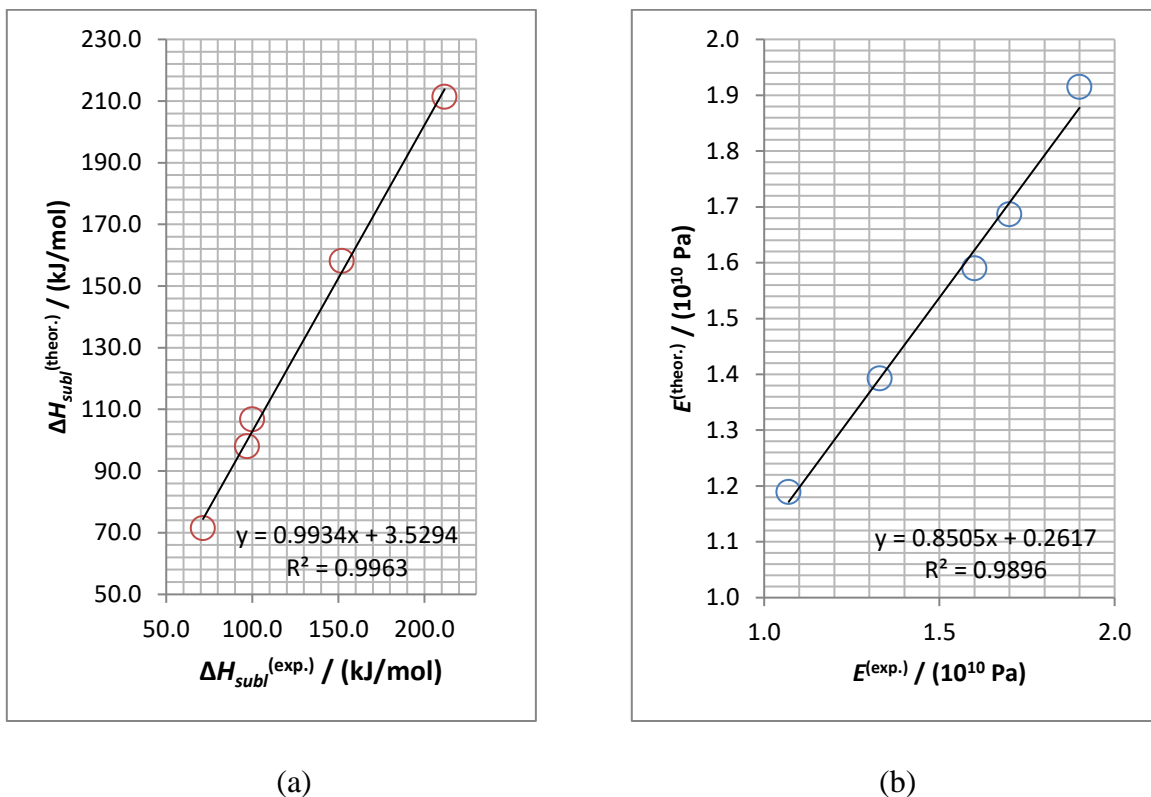
**Chart 1**

**Table 2.** Literature data and calculated values of sublimation enthalpy and Young modulus for the selected PAHs.

	$\Delta H_{sub} / (\text{kJ}\cdot\text{mol}^{-1})$ *	$E / (10^{10} \text{ Pa})$ **	$\Delta H_{sub} / (\text{kJ}\cdot\text{mol}^{-1})$ eq (22)	$E / (10^{10} \text{ Pa})$ eq (33)
Naphthalene	71.4	1.1	71.4	1.2
Anthracene	97.0	1.3	98.0	1.4
Pyrene	100.0	1.6	106.7	1.6
Coronene	152.0	1.7	158.1	1.7
Ovalene	211.7	1.9	211.4	1.9

\* from [17,40]

\*\* from [41,42]



**Figure 2.** Comparison between predicted and experimental values of (a) sublimation enthalpies and (b) Young modulus for the selected polyacenes. The linear regression is also depicted.

## 4 Discussion

The testing results indicate that the present model is reliable. It is worthy to discuss the feasibility of indirect measurement of sublimation enthalpy and Young's modulus using the present model. According to Eq (22), the thermal expansion coefficient and heat capacity are needed to determine the value of sublimation enthalpy. While the heat capacity at different temperature may be measured using a differential scanning calorimetry, which has

become a routine measurement for various organic and inorganic synthesis [43-46], the thermal expansion coefficient may be obtained through temperature-dependent X-Ray diffractometric measurements [47-51]. In order to obtain the value of Young's modulus, the internuclear/molecular distance  $r_e$  will also be needed and can be obtained from X-Ray diffraction spectroscopy. Some deviation of the predicted values from the experimentally measured data is observed for a few metallic systems; the reason might be attributed to the fact that – as said before – the interatomic potential parameters were not re-optimised for the chosen systems. In particular the choice of fixing the values of  $m$  and  $n$  in eq (4) and derived formulae might be rather critical and questionable. In order to reach a higher level of accuracy in the prediction, the potential function should be re-parameterised for each specific system, or class of systems.

## 5 Conclusions

The present work proposed a simple, yet accurate analytical model that allows to express sublimation enthalpy and Young's modulus with some conventional thermodynamic parameters, such as heat capacity and thermal expansion coefficient, along with the internuclear/molecular distance. Such model evens up the importance of sublimation enthalpy, Young's modulus and coefficient of thermal expansion, wherein no one is more important than the other, and any one of them may be determined by the other two based on their correlations. The present model not only provides a strong theoretical foundation for numerous previous work that was attempted to model the sublimation enthalpy through empirical and semi-empirical models, but also represents a useful tool, whose relevance is

immediate in the characterization of metallic, ionic and organic materials without the usage of expensive, non-conventional equipment, with remarkable repercussions in many fields of research or applications, *e.g.* food and pharmaceutical industry, environmental science, solid batteries, *etc.*

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