

**INFLUENCE OF INTERATOMIC DISTANCE CHANGE ON LINEAR DIMENSIONS OF SOLID STATE**

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The change of linear dimensions of solid material series with temperature increase and its small changes takes place and is proportional to change of distance between atoms. The harmonic oscillations don't lead to rode length change. However, the force returning atoms to balance state, lead to appearance of some anharmonicity which is described by the cube member in the expression of potential energy.

Let's consider the rode length change from solid material which increases with temperature increase. Let's designate the length increase at increase on 1K through  $(\Delta L)_1$ . Thus the thermal expansion coefficient can be defined by the following formula:

$$\tau = (\Delta L)_1 / L \tag{1}$$

which increases with temperature. If we consider the simple solid states at room temperature then coefficient change  $\tau$  can be considered as small one in the comparison with its value in the interval 100K and length increase is proportional to temperature increase  $\Delta T$ , i.e.  $\Delta L/L = \tau \Delta T$  at condition  $\Delta L \ll L$ . Let's suppose that  $\Delta L$  is proportional to  $\Delta T$  even at small length changes in order to evaluate approximately  $\tau$  coefficient value.

Let's we give such energy to the rode at which energy which is equal to energy of atom bond  $E$  (energy necessary for separation of solid state on separate atoms) is on each substance atom. Indeed, whole material is destroyed at such process. Moreover, that such destruction takes place when interatomic spaces increases in two times, i.e. rode length increases in two times ( $\Delta L=L$ ). Further, supposing that linear dependence of  $\Delta L$  on  $\Delta T$  is saved up to temperatures at which the energy  $E$  is on each atom and temperature accretion  $\Delta \tau$  is energy of measure given to each atom. For example, the temperature increase on 1 K corresponds to energy of each atom approximately on the value equal to Bolzman constant  $k$ , i.e. approximately on  $10^{-4}$  eV. According to theorem about equilibrium energy distribution on degree of freedom on 3-dimension oscillator is energy  $3 kT$ . But at investigation of rode linear extension we interest in only one direction. If linear dependence  $\Delta L$  on  $\Delta T$  takes place then extension ( $\Delta L$ ) should be less at temperature increase on 1K than extension  $\Delta L=L$  at energy obtaining by atom approximately in  $k/E$  time. Thus:

$$\tau = \frac{(\Delta L)_1}{L} \approx \frac{k}{E} \approx \frac{10^{-4}}{E} \tag{2}$$

where  $E$  is bond energy in electron-volt for substance solid state at room temperature.

The values of linear thermal expansion coefficients :  $\tau_c$  - are calculated ones,  $\tau_e$  are experimentally measured ones; the values of bond energy  $E$  and Debye parameter  $\theta$  of some substances [1,2].

Table.

Substance	$\tau_c \cdot 10^5$	$\tau_e \cdot 10^5$	$E, eV$	$\theta, K$
Na	3.9	6.9	1.1	158
Li	2.7	4.5	1.6	344
Al	1.3	2.3	3.4	428
C	0.58	0.1	7.4	2230
Fe	1.0	1.2	4.3	470
Ni	1.0	1.3	4.3	450
Si	0.94	0.25	4.6	645
Cu	1.24	1.6	3.5	450
Pb	2.2	2.9	2.0	105

As it is seen from the table many simple solid states have linear thermal expansion coefficients by  $10^{-5}$  order which is easily explained taking under consideration that temperature increase on 1K corresponds to energy which is equal to  $10^{-4} \div 10^{-5}$  bond energy, given to each atom.

The expression  $\tau = \frac{(\Delta L)_1}{L} \approx \frac{k}{E}$  is obtained on the base

of the fact that extension is proportional to temperature increase. Let's show that this supposition is carried out at small temperature changes.

Let's consider the two neighbor atoms oscillating relatively positions of their balance which is separated by distance  $d$ . We investigate the behavior of two neighbor rode atoms the material of which is characterized by interatomic spaces  $D$ . The distance between atoms is  $(d+x)$  in each time moment, where  $x$  is inclination from balance state. The oscillations are harmonic ones up to the moment when potential energy  $U_x$  can be considered as quadratic function  $U(x)=ax^2$  and average value of  $x$  is equal to zero not depending on oscillation energy value.

The harmonic oscillations are characterized by motion symmetry relatively to oscillation center that's why they don't lead to rode length change. But the force returning atoms to balance increases at  $x < 0$  and decreases at  $x > 0$ , so we can suppose the anharmonicity appearance. In comparison with harmonic motion, the strength of extension decreases at big distances between atoms and compressive strength increases at decrease of distances between them. Then in first approximation this can be described by cube member in expression for potential energy  $U(x)$ :

$$U = ax^2 - bx^3, \text{ where } a, b > 0 \tag{3}$$

At oscillation motion the kinetic energy in far points  $x_{\pm}$  are trajectories of  $x$  transform into zero. Consequently, we can make equal  $U(x)$  at  $x = x_{\pm}$  total energy. According to theorem on energy equilibrium distribution on degree of freedom, the anharmonic corrections are relatively small ones up to moment when heat energy of harmonic oscillation is equal to  $kT$ . Then we can write:

$$kT = ax_{\pm}^2 - bx_{\pm}^3 \quad (4)$$

In the case when  $b=0$ , we have  $x_{\pm} = \pm \left(\frac{kT}{a}\right)^{1/2}$ . At room temperature the cube member in potential energy is small one in the comparison with quadratic one, so we can find  $x_{\pm}$  at  $b \neq 0$  by the way of substitution of values  $x_{\pm}$  corresponding to  $b=0$  in second member of first part of expression (4):

$$x_{\pm}^2 = \frac{kT}{a} \left( 1 \pm \frac{b}{a} \sqrt{\frac{kT}{a}} \right)$$

where the root can be taken with "plus" sign. Then we define the extreme points  $x_+$  and  $x_-$  considering the second member in brackets as small one in the comparison with one, i.e.:

$$x_+ = +\sqrt{\frac{kT}{a} + \frac{b}{2a} \cdot \frac{kT}{a}} ; \quad x_- = -\sqrt{\frac{kT}{a} + \frac{b}{2a} \cdot \frac{kT}{a}}$$

Consequently, two extreme values of inclination on equilibrium are equal on absolute value and opposite on sign. They both are shifted in positive direction on the value:

$$\delta = \left(\frac{b}{2a^2}\right) \cdot kT \quad (5)$$

The average value of shift  $\bar{x}$  isn't equal to zero, but close to  $\delta$ . It isn't equal to  $\delta$  as averaging at anharmonic oscillations are enough difficult ones but we can consider  $\bar{x} \approx \delta$ .

At investigation of function behavior  $U(x)$  at  $x = d$  we can obtain the estimations for  $a$  and  $b$  parameters. In this case the approximation (3) isn't equal and we should take under consideration the members of highest orders on  $x$  in expression for potential energy. We suppose that at  $x \approx d$  the value  $U(x)$  is by the order of bond energy. And we can suppose that members of expression (3) have order by  $E$  value. Then we can consider  $a \sim E/d^2$ ;  $B \sim E/d^3$  and according to (5) we obtain the expression  $\delta/d \approx (1/2)(kT/E)$  for relative extension. As we suppose that rode length increases proportionally to distance between atoms then we obtain the following for thermal expansion coefficient:

$$\tau \approx \frac{1}{2} \frac{k}{E} \approx 0.43 \frac{10^{-4}}{E} \quad (6)$$

which coincides with formula (2). Sometimes the use of expression (2) leads to better agreement. The diamond and silicon are exclusions. This is connected with fact that Debye temperature extremely exceeds the room one. The last one means that essential part of atomic oscillations doesn't excited at room temperature and supposition on the energy  $kT$  is on each one equilibrium oscillation, isn't right. The coefficient  $\tau$  has the value  $0,51 \times 10^{-5}$  at 1400K, and for silicon  $0,45 \times 10^{-5}$  at 1200K. Consequently, formula (6) at high temperatures better corresponds to experiment.

[1] Ch. Kittel. Vvedenie v fiziku tverdogo tela. Moskva, Nauka, 1978, s. 695. (in Russian)

[2] V.F. Weiskopf, H. Bernstein. Comments Condensed Matter. Amer. J. Phys., 1985, v.53, №12, p. 38.

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### ATOMLAR ARASI MƏSAFƏNİN BƏRK CİSMİN XƏTTİ ÖLÇÜLƏRİNƏ TƏSİRİ

Göstərilmişdir ki, temperaturun artması ilə bəzi bərk cisimlərin uzunluğunun artması həqiqətən mövcuddur və temperaturun kiçik dəyişmələrinə atomlar arası məsafənin dəyişməsi ilə mütənəsbdir. Harmonik rəqslər milin uzunluğunun dəyişməsinə gətirmir. Lakin atomları tarazlıq vəziyyətinə qaytaran güvvə potensial enerjinin ifadəsində kubik həddlə ifadə olunan müəyyən anharmonizmin yaranmasına gətirir.

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### ВЛИЯНИЕ ИЗМЕНЕНИЯ МЕЖАТОМНОГО РАССТОЯНИЯ НА ЛИНЕЙНЫЕ РАЗМЕРЫ ТВЕРДОГО ТЕЛА

Изменение линейных размеров ряда твердых материалов с повышением температуры, при ее малых изменениях, действительно имеет место и пропорционально изменению расстояния между атомами. Гармонические колебания не приводят к изменению длины стержня. Однако сила, возвращающая атомы к положению равновесия, приводит к появлению некоторого ангармонизма, которое описывается кубическим членом в выражении потенциальной энергии.

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