The estimation of the internal dimensions of the channel for transport of atoms, molecules from the variation principles and the conditions of its local symmetry

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Abstract. Properties of channel in order to transport atoms (ions, molecules) is considered from point of its symmetry. Lagrange function of the transport channel is constructed. Properties of the Lagrange function and types of symmetry of the channel allow to estimate its inner size. Crystallographic channel of quartz and its dislocations are used as particular example.

1. Introduction

Variational principles, Dating back its roots to the works of Euler, Lagrange, Maupertuis [1] find wide application in modern physics, covering the research area from thermodynamics [2] and quantum physics [3,4].

One of the problems solved by L. Euler that is the problem (isoperimetric problem) search closed planar lines of finite length, which would restrict the maximum area [5].

Figure 1. Flat line L is finite and fixed length bounds the maximum area on the flat surface

The scheme is "symmetry – shape - size" arises in problems related to the movement of the atoms (molecules, ions) through channels. For the migration of foreign atoms (ions, molecules) in various bodies play a great role transport channels, the transverse dimensions of which are comparable to or exceed times the size of the transported atoms (ions, molecules) [6 – 10]. Such channels can be crystallographic channels [10] (channels with open type crystallographic structure, for example, quartz, water), dislocation [6-10], tracks from charged particles, various molecular structures in biology [9]. The evaluation of the internal size of the channel (or the core of the dislocation) can be done [10,11], but the relationship of channel structure, its symmetry and its internal diameter remains unsolved. The search for such a connection will allow to determine the effect of the channel structure on the movement of the object within the channel.

Regardless of their functional properties, the channels exhibit some properties of symmetry. Among the most common types of symmetry of the channels can distinguish cylindrical and helical symmetry.

The aim of this work is to evaluate internal dimensions (radii) of the transport channel based on its symmetry properties.
2. The model and the solution

Consider the relationship of symmetry of the channel with its inner dimensions on a particular example of crystal channel, quartz (fig.1)

Figure 2. Crystallographic channel of the quartz along the direction [0001]. Depicted oxygen ions form the “inner wall” of the channel. Each ion belongs to the structural component of the quartz - tetrahedron SiO$_4$. $R_0$ is the radius of the oxygen ion; $az$ is the projection on the z-axis distance between the centers of the oxygen ions in the channel; $h$ - period; $r$ is the distance from the axis of rotation to the center of gravity of the oxygen ion, forming a "wall" of the channel.

This channel exhibits properties of helical symmetry. To reveal these properties of symmetry, let us consider the Lagrangian $\mathcal{L}$ for a channel:

$$\mathcal{L} = \mathcal{L}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n, \varphi_1, \varphi_2, \ldots, \varphi_n)$$

Here $\vec{r}_j$ - position of $j$-th atom in the channel (Fig.1), $\varphi_j$ - rotation of the $j$-th atom along the z-axis, the upper dot marks the derivative at time $t$ from appropriate variables. The requirement of symmetry of a certain type implies the invariance of the Lagrange function relative to the variable for which the Lagrangian is preserved (Noether theorem).

At helical symmetry this means the variation of the Lagrangian $\delta \mathcal{L}$ of the channel with the translation along the z-axis ($\delta z$) and simultaneous rotation around the axis ($\delta \varphi$) equals to zero:

$$\delta \mathcal{L} = \sum_a \left( \frac{\partial \mathcal{L}}{\partial \varphi_a} \right) \delta \varphi_a + \sum_a \left( \frac{\partial \mathcal{L}}{\partial r_a} \right) \delta r_a = 0$$

(The cylindrical symmetry implies independence in relation to the transfer along the symmetry axis and the rotation about this axis

$$\delta \mathcal{L} = \sum_a \left( \frac{\partial \mathcal{L}}{\partial r_a} \right) \delta r_a = 0$$

and

$$\delta \mathcal{L} = \sum_a \left( \frac{\partial \mathcal{L}}{\partial \varphi_a} \right) \delta \varphi_a = 0$$

Variation $\delta r_a$ and $\delta \varphi_a$ for each $a$-th atom is the same, finite and arbitrary. Since each atom channel (Fig.1) is shifted by the same distance $\delta z$ and rotated by the same angle $\delta \varphi$, then

$$\sum_a \left( \frac{\partial \mathcal{L}}{\partial r_a} \right) = \delta z \sum_a \left( \frac{\partial \mathcal{L}}{\partial r_a} \right) = \delta z \sum_a \left( \frac{\partial \mathcal{L}}{\partial r_a} \right)$$

$$\sum_a \left( \frac{\partial \mathcal{L}}{\partial \varphi_a} \right) = \delta \varphi \sum_a \left( \frac{\partial \mathcal{L}}{\partial \varphi_a} \right)$$

Take into account that $\delta z = z_1 + n \cdot a_z$ then $\delta z_a = \delta (z_1 + n \cdot a_z) = \delta z$ and

$$\sum_a \left( \frac{\partial \mathcal{L}}{\partial r_a} \right) = \delta \varphi \sum_a \left( \frac{\partial \mathcal{L}}{\partial r_a} \right)$$

The same with respect to variations $\delta \varphi$:

$$\sum_a \left( \frac{\partial \mathcal{L}}{\partial \varphi_a} \right) = \delta \varphi \sum_a \left( \frac{\partial \mathcal{L}}{\partial \varphi_a} \right)$$

In this case,

$$\delta \mathcal{L} = n \left( \frac{\partial \mathcal{L}}{\partial z} \delta z + \frac{\partial \mathcal{L}}{\partial \varphi} \delta \varphi \right) = 0$$  (1)
With respect to (1) we note that the sign of the variation of a Lagrangian is not important, but the main role plays the minimum of the action $s = \int x^l \cdot f \cdot dt$ [12].

This means that the variation with positive or negative sign will inevitably lead to an increase in $s$. Therefore, the expression (1) is written in another form:

$$\delta L = n(\frac{\partial L}{\partial x}) \delta x + (\frac{\partial L}{\partial \phi}) \delta \phi = 0 \quad (1a)$$

or

$$\delta L = - (\frac{\partial L}{\partial x}) \delta x + (\frac{\partial L}{\partial \phi}) \delta \phi = 0$$

Taking into account

$$\delta x = \left(\frac{h}{2\pi}\right) \delta \phi$$

one has

$$\delta L = \frac{d}{dt} (- P_x (\frac{h}{2\pi}) + L_z) \delta \phi = 0$$

then the value

$$- P_x (\frac{h}{2\pi}) + L_z = 0 \quad (2)$$

is a conserved quantity. The constant of integration is chosen equal to zero. This eliminates uncertainty $L_z$, depending on the size of sought value $r$.

$$E_z = m^p \cdot \phi = \frac{m}{r^2} \omega$$

(3)

Note that if the variation was preserved in the form of (1), (2) would receive the complete positive form. It would lead to non-physical (imaginary) values of the radius of the channel (4), which is not good for us. Therefore, substituting (3) into (2), we obtain

$$r^2 = (m u_z \cdot \frac{h}{2\pi \omega}) = u_z \cdot \frac{h}{2\pi \omega} \quad (4)$$

$r$ means the distance from the axis of rotation of the channel to the center of gravity of the oxygen ion, forming a "wall" of the channel (Fig.2). It can be written

$$r^2 \cong \left(\frac{2\pi h}{2\pi (2\pi h)}\right) = \frac{\Delta z \cdot h}{(2\pi)}$$

Here $\Delta z$ – displacement along the axis $z$, $\tau$ – the time during which the channel would be rotated and shifted to the step $h$. Taking $\Delta z = h$, we get

$$r = \frac{h}{2\pi} \quad (4a)$$

Here it is possible to transit to the "language" of burgers vectors of $b(h = 2k)$. In the model of the channel, $\Phi_2, h = 6a$, and

$$r = \frac{h}{2\pi} \quad (5)$$

Let estimate the radius for a channel with cylindrical symmetry. It is impossible to estimate radius directly from (1) under the condition (3). (Loop should be closed). To estimate the radius of channel with cylindrical symmetry, we assume that the spiral is curved in a single step $a, i.e., h = a_x$. In this case, the minimum value of the ratio of the radius of channel with helical symmetry to the radius of the cylindrical symmetry equals

$$\left(\frac{b_0 \pi}{2\pi}\right) / \left(\frac{a_x}{2\pi}\right) = e$$

(6)

The value of the radius (of the centers of gravity of the ions forming the inner wall of the channel) for a channel with helical symmetry (Fig.2) equals to

$$r = \frac{6a_x}{2\pi} \geq 6 \cdot 1.83 \cdot 6.18 \geq 1.75 A \quad (7)$$

The radius of the cavity channel, $r - R_\phi$ (Fig.2) can be positive or negative. Here, the ion radius of the oxygen atom $R_x = (1.2 + 1.3), [13]$. Then the “radius” of the cavity of the channel for screw symmetry is equal to:

$$r_c = 1.75A - (1.2 + 1.3)A = (055 - 0.45)A \quad (8)$$

and for cylindrical symmetry we get the following value

$$r_c = \frac{a_x}{2\pi} - (1.2 + 1.3)A \approx - (0.9 + 1.0)A \quad (9)$$
From comparison of relations (8) and (9) of the radii of the channels for screw and cylindrical symmetry it follows that the channel with cylindrical symmetry is covered with oxygen ions is much stronger than the channel with helical symmetry, as can be seen in figure 3.

Figure 3. The overlap of the ionic radii of oxygen crystallographic channel: a) helical symmetry and b) with cylindrical symmetry. The dotted line indicates the blocked part of the channel. $R_0$ is the radius of the oxygen ion; $r_n$ is the radius of channel with helical symmetry; $r_c$ is the radius of channel with cylindrical symmetry.

This implies that in a channel with helical symmetry "free space" for the placement of foreign atom more than in a channel with cylindrical symmetry. Minimum screw dislocation (providing the minimum elastic energy) in quartz are located along the crystallographic channels by stretching or compressing them [10]. Distance $a_x$ (7) and (9) along the z-axis of "expanded" channel is changed $a_x = \frac{3}{2}a_x$. The ratio (6) will not change, but the radii of the cavities (8) and (9) for both helical and cylindrical symmetry will change as follows:

1) for the core of the dislocation with screw symmetry the radius of the distance of the centers of gravity of the oxygen ions from the z axis is equal to $r = 2.65\text{Å}$ the radius of the cavity

$$r_n = \frac{3}{2}a_x - (1.2 + 1.3)\text{Å} = (1.425 + 1.325)\text{Å}.$$

2) for the same channel in the approximation of cylindrical symmetry associated radii equal to:

$$r_c = \frac{3}{2}a_x - \frac{3\pi}{2} - (1.1 + 1.3)\text{Å} = 0.291\text{Å} - (1.2 + 1.3)\text{Å} = -(0.763 + 0.063)\text{Å}.$$

Grown nanotubes [15] have demonstrated properties of the cylindrical and helical symmetry too and have different radii

Figure 4. Nanotubes a) without dislocation (cylindrical symmetry), b) with dislocation (helical symmetry)

3. Conclusion
The work was able to show, explicitly, the influence of the type of the local symmetry of the transport channel at its inner radius of the cavity. It turned out that the channel with helical symmetry has an internal radius substantially greater than the radius of the channel with cylindrical symmetry. Since the clarification of connection of local symmetry with form and size of channel was used General principles of minimum of action, it can be assumed that, in most cases, the organization of transport channels for the transfer of atoms (molecules, ions) preferred type of symmetry is the structure of the channel showing the properties of helical symmetry.
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