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# An improvement of the lattice theory of dislocation for a two-dimensional triangular crystal*

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The structure of dislocation in a two-dimensional triangular crystal has been studied theoretically on the basis of atomic interaction and lattice statics. The theory presented in this paper is an improvement to that published previously. Within a reasonable interaction approximation, a new dislocation equation is obtained, which remedies a fault existing in the lattice theory of dislocation. A better simplification of non-diagonal terms of the kernel is given. The solution of the new dislocation equation asymptotically becomes the same as that obtained in the elastic theory, and agrees with experimental data. It is found that the solution is formally identical with that proposed phenomenologically by Foreman *et al*, where the parameter can be chosen freely, but cannot uniquely determined from theory. Indeed, if the parameter in the expression of the solution is selected suitably, the expression can be well applied to describe the fine structure of the dislocation.

**Keywords:** dislocation, lattice theory, triangular lattice
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Dislocation is a kind of structural defects that are believed to be the origin of solid plasticity. Generally, dislocation can be understood as a topological defect existing in an ordered phase. In nature, the two-dimensionally ordered phase mostly occurs in the form of triangular lattice. The reason is that the triangular lattice is the only close-packed structure in two-dimensional space and thus has a relatively low ground energy. The dislocation had been studied extensively in the past decades. Unfortunately, there is still not a fully discrete theory of dislocation based on atomic interaction and lattice statics. Maradudin's model was the first atomic model of dislocation.[1] However, in Maradudin's model, dislocation results from a source that is given phenomenologically and can hardly be obtained self-consistently. Peierls' model provides in principle a scheme to deal with dislocation systematically from the atomic interaction and fundamental equation.[2,3] In Peierls' model, the crystal containing dislocations is first divided adequately into two perfect parts in which atoms align regularly; and then dislocation is produced through non-linear interaction between the two parts. However, in order to gain dislocations analytically by using Peierls' scheme, one has to solve the deformation problem of a half-infinite crystal to which a given force is applied on the border. This is a difficult problem that greatly limits the application of Peierls' scheme. In the well-known Peierls model, the problem is solved by approximating the crystal as an elastic continuum medium.[2−4] Recently, the author of this paper developed a method to deal with the half-infinite problem, and successfully obtained an analytical solution for a two-dimensional triangular lattice. This result has been used to establish a full lattice theory of dislocation, including deriving a dislocation equation and calculating the dislocation structure.[5,6] In this paper, a substantial improvement to the lattice theory of dislocation is presented. Firstly, based on the solution of the half-infinite problem, a new dislocation equation is derived, which remedies a fault that existed in the lattice theory given before. Secondly, a better simplification to the kernel $\Lambda$ is obtained, which can lead to correct asymptotic behaviour in the area far from the core of the dislocation. Thirdly, a well-approximated solution of the dislocation equation is discussed, which is surprisingly identical with that proposed phenomenologically by Foreman *et al*[7] for the horizontal displacement. Besides, the force-law used widely in the analytical theory of dislocation is explained by means of the phase concept.

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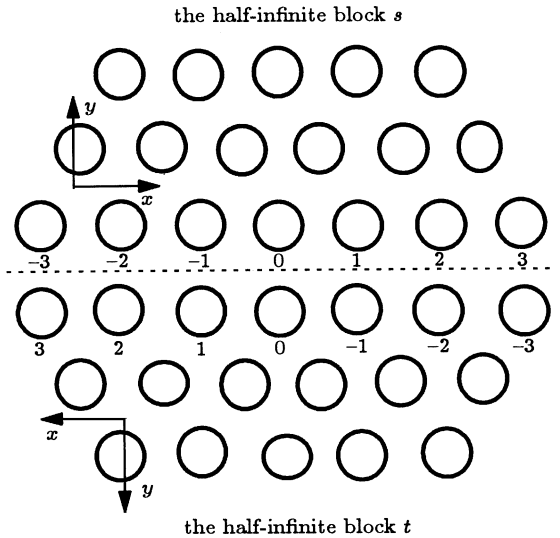



**Fig.1.** The reference configuration of the atoms and the local frames given by a pair of orthogonal unit vectors $x$ and $y$. The crystal is divided into an upper part and a lower part along the dotted line. The displacement given in the text is relative to the position in this figure.

For a two-dimensional triangular crystal, by using the solution of the half-infinite lattice which is acted upon by a given force on the border,[5] the dislocation equation that only relates to the atoms on the borders, through which the two perfect crystals match together, can be written as

$$\sum_{\ell'} \Lambda(\ell-\ell')\boldsymbol{u}^s(\ell') = \boldsymbol{f}^s(\ell),$$
$$\sum_{\ell'} \Lambda(-\ell+\ell')\boldsymbol{u}^t(-\ell') = \boldsymbol{f}^t(-\ell), \tag{1}$$

where the column vector $\boldsymbol{u}^s$ ($\boldsymbol{u}^t$) is the displacement of the border atoms, and column vector $\boldsymbol{f}^s$ ($\boldsymbol{f}^t$) is the force exerted by the atoms on different borders. Superscripts $s$ and $t$ are used to distinguish the upper part and lower part respectively. The $2\times 2$ matrix $\Lambda(\ell)$ is given by [5]

$$\Lambda(\ell) = \frac{(-1)^\ell}{\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}q\tilde{\Lambda}(q)\mathrm{e}^{-\mathrm{i}2\ell q}, \tag{2}$$

$$\tilde{\Lambda}(q) = \begin{bmatrix} 1+\cos 2q + \dfrac{2(1+\cos 2q)\sqrt{\zeta\zeta^*}}{\sqrt{\zeta}\mathrm{e}^{-\mathrm{i}q}+\sqrt{\zeta^*}\mathrm{e}^{\mathrm{i}q}} & -\dfrac{\sqrt{3}\cos q(\sqrt{\zeta}-\sqrt{\zeta^*})}{\sqrt{\zeta}\mathrm{e}^{-\mathrm{i}q}+\sqrt{\zeta^*}\mathrm{e}^{\mathrm{i}q}} \\ \dfrac{\sqrt{3}\cos q(\sqrt{\zeta}-\sqrt{\zeta^*})}{\sqrt{\zeta}\mathrm{e}^{-\mathrm{i}q}+\sqrt{\zeta^*}\mathrm{e}^{\mathrm{i}q}} & \dfrac{3}{2}\dfrac{(1+\cos 2q)}{\sqrt{\zeta}\mathrm{e}^{-\mathrm{i}q}+\sqrt{\zeta^*}\mathrm{e}^{\mathrm{i}q}} \end{bmatrix} \tag{3}$$

with

$$\zeta = 1+\frac{1}{4}\mathrm{e}^{\mathrm{i}2q}, \qquad -\frac{\pi}{2}\le q\le\frac{\pi}{2},$$

where the harmonic interaction constant has been taken to be unity. In order to use the same kernel $\Lambda$ for both upper and lower half-infinite crystals, it is necessary to use a local coordinate system that is intrinsic to the crystal block (see Fig.1). Obviously, if the upper part rotates $180^o$, it will change into the lower part. Therefore, the intrinsic coordinates differ only a minus sign for the two atoms that change into each other through rotating $180°$. In Ref.[5], regretfully, the same kernel $\Lambda$ was used for both upper and lower parts without making a coordinate transformation. As shown in the following, the previous statement that the centre of mass of the paired atoms was fixed is valid only when the vertical displacement is negligible. If the vertical displacement is taken into account, one only has the fixed horizontal position of the centre of mass.

Equation (1) is the exact equation for dislocation, but it is too complicated to be solved. In order to make a simplification, we introduce mass-centre displacement $\boldsymbol{u}^c(\ell)$ and relative displacement $\boldsymbol{u}^r(\ell)$ for a pair of atoms labelled by $\ell$ and $-\ell$,

$$\boldsymbol{u}^r(\ell) = \frac{1}{2}[\boldsymbol{u}^s(\ell)+\boldsymbol{u}^t(-\ell)],$$
$$\boldsymbol{u}^c(\ell) = \frac{1}{2}[\boldsymbol{u}^s(\ell)-\boldsymbol{u}^t(-\ell)],$$

where $\boldsymbol{u}^r$ is actually the displacement relative to the centre of mass, and split the kernel $\Lambda(\ell)$ into even-part $\Lambda^{(\mathrm{e})}(-\ell)=\Lambda^{(\mathrm{e})}(\ell)$ and odd-part $\Lambda^{(\mathrm{o})}(-\ell)=-\Lambda^{(\mathrm{o})}(\ell)$ in respect of discrete variable $\ell$,

$$\Lambda(\ell) = \Lambda^{(\mathrm{e})}(\ell)+\Lambda^{(\mathrm{o})}(\ell).$$

From the expression of $\Lambda$ given above, it can be proved that $\Lambda^{(\mathrm{e})}$ is a diagonal matrix and $\Lambda^{(\mathrm{o})}$ is an asymmetrical matrix

$$\Lambda^{(\mathrm{e})} = \begin{bmatrix} \Lambda_{11} & 0 \\ 0 & \Lambda_{22} \end{bmatrix},$$

$$\Lambda^{(\mathrm{o})} = \begin{bmatrix} 0 & \Lambda_{12} \\ -\Lambda_{12} & 0 \end{bmatrix}.$$

The non-diagonal elements of matrix $\Lambda$ represent an induced effect while the diagonal elements represent a

direct effect that plays a dominant role. In terms of $\boldsymbol{u}^r(\ell)$ and $\boldsymbol{u}^c(\ell)$, Eq.(1) becomes

$$\begin{aligned}&\sum_{\ell'}[2\Lambda^{(\mathrm{e})}(\ell-\ell')\boldsymbol{u}^r(\ell')+2\Lambda^{(\mathrm{o})}(\ell-\ell')\boldsymbol{u}^c(\ell')]\\ =&\boldsymbol{f}^s(\ell)+\boldsymbol{f}^t(-\ell),\\ &\sum_{\ell'}[2\Lambda^{(\mathrm{e})}(\ell-\ell')\boldsymbol{u}^c(\ell')+2\Lambda^{(\mathrm{o})}(\ell-\ell')\boldsymbol{u}^r(\ell')]\\ =&\boldsymbol{f}^s(\ell)-\boldsymbol{f}^t(-\ell).\end{aligned}\tag{4}$$

Generally, the total force experienced by a pair of atoms is negligible

$$\boldsymbol{f}^s(\ell)-\boldsymbol{f}^t(-\ell)\approx 0,\tag{5}$$

where the minus appears due to different coordinate systems being used separately for the upper and lower parts. Furthermore, it is reasonable to assume that if the interval between the upper border and lower border is kept at its equilibrium value, the force that bring about the horizontal displacement lies approximately in the horizontal direction. In other words, the vertical component of the force is negligible if the vertical relative displacement vanishes,

$$f_y^s(\ell)+f_y^t(-\ell)\approx 0,\quad \text{as}\quad u_y^r(\ell)\longrightarrow 0.\tag{6}$$

Within the approximations of Eqs.(5) and (6), it is easy to prove that one can obtain a dislocation solution with no vertical relative-displacement and no horizontal movement of the centre of mass,

$$u_y^r(\ell)=0,\qquad u_x^c(\ell)=0.$$

In fact, this is the physical solution that we want because it degenerates into Peierls one[2] when the vertical displacement is neglected. The two paired atoms without vertical relative-displacement have the same vertical displacement

$$u_y^s(\ell)=-u_y^t(-\ell)=u_y^c(\ell).\tag{7}$$

The two paired atoms without horizontal movement of the centre of mass have the horizontal displacements that are equal in magnitude, but opposite in direction

$$u_x^s(\ell)=u_x^t(-\ell)=u_x^r(\ell).\tag{8}$$

It should be noted that Eqs.(7) and (8) are given in the local coordinate systems shown in Fig.1. By using Eqs.(7) and (8), from Eq.(4) one can obtain the equation satisfied by $u_x^s(\ell)$ and $u_y^s(\ell)$

$$\begin{aligned}&\sum_{\ell'}[\Lambda_{11}(\ell-\ell')u_x^s(\ell')+\Lambda_{12}(\ell-\ell')u_y^s(\ell')]=f_x^s(\ell),\\ &\sum_{\ell'}[\Lambda_{22}(\ell-\ell')u_y^s(\ell')-\Lambda_{12}(\ell-\ell')u_x^s(\ell')]=0.\end{aligned}\tag{9}$$

Equation (9) is a satisfactory equation of dislocation that has remedied the fault occurring before, and that can be a reasonable starting point in the discussion of dislocation structure.

The interaction between atoms on the neighbouring borders is crucial for a model of dislocation. In the discussion of dislocation, as first proposed by Frenkel and Kontorova,[8] one can assume that from the "eye" of the atom, the alignment of the atoms on the opposite border is nearly the same as that in a perfect crystal but a translation. That is to say, each individual atom feels a periodic potential $\phi$ resulting from the atoms on the other border,

$$\phi[\boldsymbol{u}^s(\ell)+\boldsymbol{u}^t(-\ell)+\ell_1\boldsymbol{a}_1]=\phi[\boldsymbol{u}^s(\ell)+\boldsymbol{u}^t(-\ell)].$$

And the periodic potential is the same for every atom except for a phase shift. The total interaction is the summation over all the atoms on one border

$$\sum_{\ell}\phi[\boldsymbol{u}^s(\ell)+\boldsymbol{u}^t(-\ell)].\tag{10}$$

Note that $\phi$ can be calculated explicitly if the interaction between atoms is known.

Obviously, the total force experienced by a pair of atoms labelled by $\ell$ and $-\ell$ will vanish when the force law is given by Eq.(10). The periodic potential $\phi$ can be expanded in Fourier series. If the leading term is kept only in approximation, one has the sinusoidal-force law

$$f_\ell^x=\frac{a}{4\pi}\sin\frac{4\pi u_\ell^x}{a},\tag{11}$$

where $a$ is the lattice constant.

In order to evaluate the structure of dislocation explicitly, it is necessary to make a simplification for the kernel $\Lambda(\ell)$. In Ref.[5], a simplification of the kernel $\Lambda(\ell)$ was presented. However, that simplification for the non-diagonal terms is not as good as that for the diagonal terms. A better one, which can correctly express an asymptotic behaviour, is

$$\Lambda(\ell)=\begin{bmatrix}\dfrac{3}{4}(2\delta_\ell-\delta_{\ell+1}-\delta_{\ell-1})+\dfrac{4}{\sqrt{3}\pi}\dfrac{1}{1-4\ell^2} & \dfrac{4}{3\sqrt{3}}\dfrac{c_\ell\mathrm{sgn}(\ell)}{\ell!8^\ell}\\ -\dfrac{4}{3\sqrt{3}}\dfrac{c_\ell\mathrm{sgn}(\ell)}{\ell!8^\ell} & \dfrac{8}{3\pi}\dfrac{1}{1-4\ell^2}\end{bmatrix},\tag{12}$$

where $\delta_\ell$ is the delta-function, $\delta_\ell = 1$ if $\ell = 0$, $\delta_\ell = 0$ if $\ell \neq 0$, $\mathrm{sgn}(\ell)$ is the sign-function, $\mathrm{sgn}(\ell) = 1$ if $\ell > 0$, $\mathrm{sgn}(\ell) = -1$ if $\ell < 0$, $\mathrm{sgn}(\ell) = 0$ if $\ell = 0$, $c_\ell = 1 \times 3 \times 5 \times \cdots \times (2\ell - 3)$ and $c_1 = 1$.

Because the deformation related to a dislocation varies slowly, as in Ref.[5], one can reasonably change the dislocation equation into an integral-differential equation by using the following relations:

$$\begin{aligned}
&\sum_{\ell'} \frac{u_x^s(\ell')}{1 - 4(\ell - \ell')^2} \\
&= \int_{-\infty}^{\infty} \frac{u_x^s(x')a^2}{a^2 - 4(x - x')^2} \frac{\mathrm{d}x'}{a} \\
&= -\frac{1}{4} \int_{-\infty}^{\infty} \left[ \frac{u_x^s(x')}{x' - x - \frac{a}{2}} - \frac{u_x^s(x')}{x' - x + \frac{a}{2}} \right] \mathrm{d}x' \\
&= -\frac{1}{4} \int_{-\infty}^{\infty} \frac{u_x^s(x' + \frac{a}{2}) - u_x^s(x' - \frac{a}{2})}{x' - x} \mathrm{d}x' \\
&= -\frac{a}{4} \int_{-\infty}^{\infty} \frac{\frac{\mathrm{d}u_x^s}{\mathrm{d}x'}}{x' - x} \mathrm{d}x', \qquad (13)
\end{aligned}$$

$$\begin{aligned}
&\sum_{\ell'} \Lambda_{12}(\ell - \ell') u_y^s(\ell') \\
&= \sum_{\ell' > 0} \Lambda_{12}(\ell') [u_y^s(\ell - \ell') - u_y^s(\ell + \ell')] \\
&= \sum_{\ell' > 0} (-2\ell') \Lambda_{12}(\ell') \frac{\mathrm{d}u_y^s}{\mathrm{d}x} a = -\frac{2}{9} a \frac{\mathrm{d}u_y^s}{\mathrm{d}x}, \qquad (14)
\end{aligned}$$

where $x = \ell a$. Note that the numerical factor in front of the derivative in Eq.(14) differs slightly from that given in Ref.[15].

The dislocation equation (9) now can be written as

$$\begin{aligned}
&-\frac{3}{4} \frac{\mathrm{d}^2 u_x^s}{\mathrm{d}x^2} - \frac{2}{9} \frac{\mathrm{d}u_y^s}{\mathrm{d}x} \\
&- \frac{1}{\sqrt{3}\pi} \int_{-\infty}^{\infty} \frac{\frac{\mathrm{d}u_x^s}{\mathrm{d}x}|_{x=x'}}{x' - x} \mathrm{d}x' = \frac{1}{4\pi} \sin(4\pi u_x^s), \\
&\frac{2}{9} \frac{\mathrm{d}u_x^s}{\mathrm{d}x} - \frac{2}{3\pi} \int_{-\infty}^{\infty} \frac{\frac{\mathrm{d}u_y^s}{\mathrm{d}x}|_{x=x'}}{x' - x} \mathrm{d}x' = 0, \qquad (15)
\end{aligned}$$

where the displacement and coordinates are measured in units of lattice constant. The relevant boundary condition is

$$u_x^s|_{x \to \pm\infty} = \pm \frac{1}{4}, \qquad (16)$$

Even for the integral-differential equation (15), it is hard to solve rigorously. A method for perturbatively obtaining dislocation solution of Eq.(15) has been developed by introducing a new family of orthogonalized polynomials.[6] The final solution is

$$\begin{aligned}
u_x^s &= \pm \frac{1}{2\pi} \left( \arctan p + \frac{cp}{1 + p^2} \right), \\
u_y^s &= \mp \frac{1}{12\pi} \left[ \ln(1 + p^2) + \frac{2cp^2}{1 + p^2} \right], \qquad (17)
\end{aligned}$$

with

$$c = 0.76, \qquad p = \kappa x, \qquad \kappa = \frac{\sqrt{3}(1 - c)}{1 - \frac{2\sqrt{3}}{27}}.$$

The expression of the horizontal displacement is similar to that given in Ref.[5], but the parameters $c$ and $\kappa$ are different. In Fig.2, the horizontal displacement obtained here is compared with previous one. The change is not large due to the effect of the vertical deformation, which cancels the change brought about from new treatment. However the result is in good agreement with experimental data as quoted in Ref.[7]. The vertical displacement, which becomes the same as that given in the elastic theory in the area far from the core of dislocation, is analytically obtained for the first time. It varies slowly, but diverges logarithmically. It can be observed in large-scale measurement.

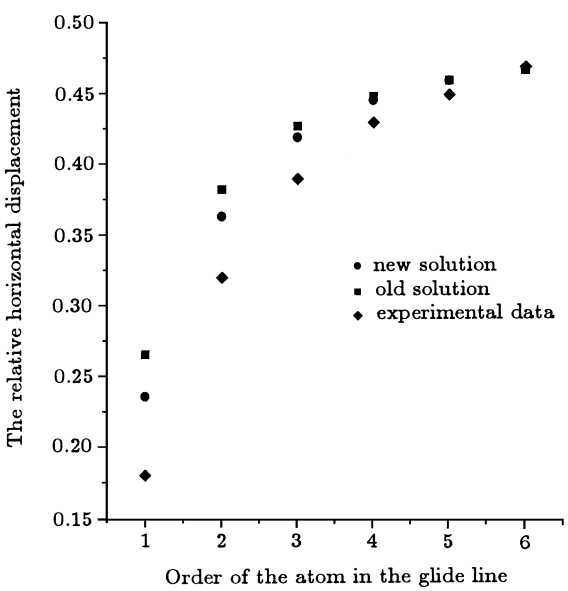



**Fig.2.** The relative displacement $2u_x^s$ of the paired atoms on the borders. Circles represent the new solution obtained in this paper, squares represent the old solution. Diamonds represent the experimental data for bubbles of 1.3mm in diameter. The atom at the centre of dislocation remains fixed. Obviously, the old theoretical result has been improved.

The dislocation structure described by Eq.(17) is close to that observed in experiment.[9] However, the

error exists in particular near the centre of the dislocation. In order to have a precise theoretical prediction, it is necessary to make a modification to the harmonic approximation, sinusoidal force-law, etc. In particular, it should be explained why the dislocation structure in the bubble raft depends on the radius of bubble. The challenge of making precise prediction is tremendous if one wants to solve the problem systematically. Nevertheless, it is worth pointing out that dislocation structure can be uniformly described by Eq.(17) provided that different parameter $c$ is chosen in different cases. In Table 1, displacements for bubbles of 1.3mm diameter are listed. As indicated, the values of $u_x|_{\rm fit}$ given by fitting agree well with the experimental data. This is meaningful because it implies that, in a sense, the structure of dislocation is controlled only by a single parameter. All the modifications to the current model can be attributed to a change of the parameter $c$.

**Table 1.** The relative displacements of the atoms labelled by $\ell$ and $-\ell$.

| $\ell$ | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| $2u_x\|_{\rm exp}$ | $1.8\times10^{-1}$ | $3.2\times10^{-1}$ | $3.9\times10^{-1}$ | $4.3\times10^{-1}$ | $4.5\times10^{-1}$ |
| $2u_x\|_{\rm Foreman}$ | $2.0\times10^{-1}$ | $3.2\times10^{-1}$ | $3.9\times10^{-1}$ | $4.3\times10^{-1}$ | $4.6\times10^{-1}$ |
| $2u_x\|_{\rm fit}$ | $1.9\times10^{-1}$ | $3.2\times10^{-1}$ | $3.9\times10^{-1}$ | $4.3\times10^{-1}$ | $4.5\times10^{-1}$ |
| $2u_x\|_{c=0.76}$ | $2.4\times10^{-1}$ | $3.6\times10^{-1}$ | $4.2\times10^{-1}$ | $4.5\times10^{-1}$ | $4.6\times10^{-1}$ |
| $u_y\|_{c=0.76}$ | $-1.3\times10^{-2}$ | $-3.6\times10^{-2}$ | $-5.7\times10^{-2}$ | $-7.2\times10^{-2}$ | $-8.5\times10^{-2}$ |

The values of $u_x|_{\rm exp}$ and $u_x|_{\rm Foreman}$ are respectively taken from experimental measurement and Foreman's phenomenological model,[7] $u_x|_{c=0.76}$ and $u_y|_{c=0.76}$ are the solution of the dislocation equation (15), the value of $u_x|_{\rm fit}$ is evaluated from Eq.(17) where the parameter $c$ is chosen to be 0.82 for fitting.

It is interesting to note that the expression of the horizontal displacement is identical with Foreman's phenomenological one[7] if the parameter $c$ is replaced by a new one defined by $a = 1/(1-c)$. But the physical origination is quite different. Foreman's one originates from the modification to the force law, while the present one originates from the discreteness.

In summary, based on the solution of the half-infinite problem, a new dislocation equation is obtained within a reasonable interaction approximation. The equation obtained remedies a fault taking place in Ref.[15]. With the improved simplification of the kernel, the equation can serve as a good starting point in the theoretical investigation of the dislocation structure. The agreement between the solution of the equation and the experimental data is much better than Peierls' one. If the parameter in the expression of the solution is selected suitably, the expression (17) can be well applied to describe the fine structure of the dislocation.

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