THEORY OF DYNAMIC DEFORMATIONS OF CRYSTAL LATTICES

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We use the harmonic approximation of crystal-lattice dynamics to solve the equations of motion of the atoms of a crystal having a complex lattice for the following initial conditions: all the crystal atoms are at the lattice nodes; the two semibounded parts of the crystal obtained by dividing the latter by an arbitrary crystal plane have velocities normal to this plane which are equal in magnitude but opposite in direction. From the resulting solution we identify the macroscopic components—step sublattice uniform deformation waves and step shear waves of the sublattices relative to one another; the connection between their amplitudes is established. It is shown that the microscopic solution differs from the macroscopic in the finite dimensions of the shock wave front. In the course of time the dimension of the region occupied by the wave front increases as $t^{1/3}$; but the ratio of this quantity to the distance traveled by the wave tends to zero in the course of time. It is established that the kinetic energy of colliding crystals is completely transformed into "elastic" energy [1] and thermal vibrations of the atoms are not excited.

1. Simple initial conditions. In this section we obtain the solutions of the equations of motion of a complex lattice for certain simple initial conditions. This is necessary in order to make it possible to generalize the problem of the collision of two semibounded crystals [2] to the case of a complex lattice. Thus we let the complex lattice consist of p + 1 simple sublattices ($\nu = 0, 1, 2, ..., p$). One of them ($\nu = 0$) is called the basic sublattice. Following [2] it can be broken down into a system of equidistant crystal planes and we can introduce the system of basis vectors and the coordinate reference system. The radius vector of an arbitrary lattice node will be

$$\mathbf{r}_{n\nu} = \mathbf{r}_{0} + \mathbf{r}_{\nu} = n_{1}\mathbf{a}_{1} + n_{2}\mathbf{a}_{2} + n_{3}\mathbf{a}_{3} + \mathbf{r}_{\nu}$$
(1.1)

The symbol n_3 now numbers not only the crystal planes of the basic sublattice but also the parallel planes of the other sublattices. Without limiting generality we can assume that the plane numbers increase in the positive direction of the x_3 -axis, and between the two planes $n_3 = N$ and $n_3 = N + 1$ of the basic sublattice there are located p planes of the other sublattices, each with the number $n_3 = N$.

Let the initial conditions be

$$u_{n \vee i}(0) = 0, \ \dot{u}_{n \vee i}(0) = v \delta_{n m} \delta_{\nu \mu} \delta_{i j} \tag{1.2}$$

where $u_n v_i(t)$ is the displacement from the equilibrium position of the plane with number n of sublattice v in the direction of the x_i -axis. Since this problem is that of the motion of a chain of planes, its solution is sought in the form of the superposition of harmonic plane waves whose wave vectors are perpendicular to the planes

$$u_{nvi}(\mathbf{k}, t) = e_{vi}(\mathbf{k}) \exp i \left[\mathbf{kr_n} \pm \omega(\mathbf{k}) t \right]$$

$$u_{nvi}(q) = e_{vi}(q) \exp i \left[nq \pm \omega(q) t \right], \ \mathbf{k} = q\mathbf{b}_3$$
(1.3)

where the amplitudes $e_{\nu i}(\mathbf{k})$ are the solutions of the dynamic equations

$$\sum_{\mu, j} \{B_{\nu i\mu j}(\mathbf{k}) - M_{\mu} \delta_{\mu\nu} \delta_{ij} \omega^{2}(\mathbf{k})\} e_{\mu j}(\mathbf{k}) = 0$$

$$B_{\nu i\mu j}(\mathbf{k}) = \sum_{\mathbf{m}} \Phi_{\mathbf{n}\nu i\mathbf{m}\mu j} \exp i\mathbf{k} (\mathbf{r}_{\mathbf{m}} - \mathbf{r}_{\mathbf{n}})$$
(1.4)

 $\Phi_{n \nu i m \mu j}$ are the lattice force constants. Hence (for more detail see [3], p. 29)

$$B_{\nu i\mu j}(\mathbf{k}) = B_{\nu i\mu j}(-\mathbf{k}), \quad e_{\nu i}(\mathbf{k}) = e_{\nu i}(-\mathbf{k})$$
(1.5)

i.e., the real parts of these quantities are even functions of k, the imaginary parts are odd and therefore approach zero as $|\mathbf{K}| \rightarrow 0$. Now we can obtain the solution of the problem with the initial conditions (1.2)

$$u_{nvi}(t) = \sum_{s=1}^{3(p+1)} \frac{v}{2\pi} \int_{-\pi}^{\pi} \frac{M_{\mu} e_{(s)\,\mu j}(q) e_{(s)\,v i}(q)}{M_{\omega_{(s)}}(q)} e^{i(n-m)q} \sin\left[\omega_{(s)}(q)\,t\right] dq$$
(1.6)

Here s is the number of the spectrum branch and $M = \sum_{\nu} M_{\nu}$ is the cell mass.

Here, in contrast with formula (2.8) in [2], we have used the following normalizing relations to simplify the result

$$\sum_{s} e_{(s)\mu j}(\mathbf{k}) e_{(s)\nu i}(\mathbf{k}) \frac{M_{\mu}}{M} = \delta_{\nu \mu} \delta_{ij}, \quad \sum_{\nu, i} e_{(s)\nu i}(\mathbf{k}) e_{(r)\nu i}(\mathbf{k}) \frac{M_{\nu}}{M} = \delta_{sr}$$
(1.7)

2. Collision of two semibounded crystals; sublattice deformations. To obtain the solution of the problem of the collision of two semibounded crystals [2], we first solve the problem with the initial conditions

$$u_{n\nu i}(0) = 0, \quad u_{n\nu i}(0) = -\nu \delta_{i3}, \quad (0 \le n \le N - 1)$$
$$u_{n\nu i}(0) = \nu \delta_{i3}, \quad (-N \le n \le -1), \qquad u_{n\nu i}(0) = 0 \quad (n < -N, n > N - 1)$$

and then $N \rightarrow \infty$, hence

$$u_{n\nu i}(t) = -\sum_{s, \mu} \frac{M_{\mu}v}{M\pi} \int_{0}^{\pi} \left\{ \operatorname{Im} \left[e_{(s)\mu 3}(q) e_{(s)\nu i}(q) \right] \frac{\cos\left(n + \frac{1}{2}\right)q}{\sin^{1}/2q} + \operatorname{Re} \left[e_{(s)\mu 3}(q) e_{(s)\nu i}(q) \right] \frac{\sin\left(n + \frac{1}{2}\right)q}{\sin^{1}/2q} \right\} \frac{\sin\left[\omega_{(s)}(q)t\right]}{\omega_{(s)}(q)} dq$$
(2.1)

Here we have used solution (1.6), the second relation of (1.5), and also the fact that

$$\int_{0}^{\pi} f(q) \cos Nq \, dq \to 0 \quad \text{as } N \to \infty$$

if f(q) is a function which is continuous on the interval $[0, \pi]$. From (2.1) we can obtain the quantities

$$\sigma_{nvi}(t) = \frac{1}{a} \left[u_{nvi}(t) - u_{n+1vi}(t) \right], \quad a = \frac{1}{|\mathbf{b}_3|}$$

$$\kappa_{nv\mu i}(t) = \left[u_{nvi}(t) - u_{n\mu i}(t) \right]$$
(2.2)

Here a is the distance between closest planes of a single sublattice

$$\sigma_{nvi}(t) = \sum_{s, \mu} \frac{2vM_{\mu}}{a\pi M} \left\{ \int_{0}^{\pi} \operatorname{Im} \left[e_{(s)\mu3}(q) \ e_{(s)vi}(q) \right] \frac{\sin \left[\omega_{(s)}(q) \ t \right]}{\omega_{(s)}(q)} \sin nq \ dq - - \int_{0}^{\pi} \operatorname{Re} \left[e_{(s)\mu3}(q) \ e_{(s)vi}(q) \right] \frac{\sin \left[\omega_{(s)}(q) \ t \right]}{\omega_{(s)}(q)} \cos nq \ dq \right\}$$
(2.3)

Using the method of stationary phase [2, 4, 5], we can see that undamped disturbances are contained only in the integrals of the lower line of (2.3) and only in those in which $\omega_{(S)}(q) \rightarrow 0$ as $q \rightarrow 0$, i.e., only for the three acoustic spectrum branches s = 1, 2, 3. Separating the undamped disturbances and taking into account the relation which will be obtained later in the paper

$$e_{(s)vi}(0) = e_{(s)\mu i}(0) = e_{(s)i}(0) \qquad (s = 1, 2, 3)$$
(2.4)

we can obtain three step-function uniform-deformation waves for each sublattice:

$$\sigma_{(s)vi}(t, n) \approx \sigma_{(s)i}(t, n) \equiv \begin{cases} -e_{(s)3}(0) e_{(s)i}(0) v/c_{(s)}, c_{(s)t} > na \\ 0 & c_{(s)t} < na \\ s = 1, 2, 3 \end{cases}$$

Here $c_{(S)}$ is the speed of sound.

The solution of the problem of propagation of disturbances caused by the action on one of the crystal planes of an external force having the form of a square pulse can be obtained from (1.6). In both cases the microscopic picture, just as in the case of the simple lattice, is characterized by damped disturbances. In the complex lattice, among them

there will be disturbances having the frequencies of the optical branches of the spectrum, including the disturbances associated with the inflection points of these branches. The latter decay in time as $t^{-1/3}$.

3. Shock wave front. Now we can see that in the complex lattice case, just as in the simple lattice case [2], the shock waves which arise upon collision of two semibounded crystals are described by integrals of the form

$$J(\tau, n) = \int_{0}^{\pi} \frac{\psi(q)}{q} \sin \left[\tau \varphi(q)\right] \cos nq \, dq \quad \left(\tau = \frac{ct}{a}\right) \tag{3.1}$$

Here τ is dimensionless time; c is the sound speed for the acoustic spectrum branch in question; $\psi(q)$ and $\varphi(q)$ are functions which have a sufficient number of continuous derivatives on the interval $[0, \pi]$, and as $q \rightarrow 0$

$$\varphi(q) \approx q + \frac{\varphi^{m}(0)}{3!} q^3 + \frac{\varphi^{9}(0)}{5!} q^5, \quad \psi(q) \approx \psi(0) + \frac{\psi^{n}(0)}{2!} q^2$$
(3.2)

The macroscopic approximation of (5.1) is the step wave

$$J(\tau, n) \approx \begin{cases} 1/2 \ \psi(0) \ \pi, & \tau > n \\ 0, & \tau < n \end{cases}$$
(3.3)

To study integral (3.1) in more detail for $\tau \approx n$, i.e., near the shock wave front, it is sufficient to set in (3.1) $\tau = N$, where $N \gg 1$, and n = N + l, where $l \ll N$. Hence

$$J(\tau, n) = J(N,l) \equiv J_{1(+)}(N, l) + J_{1(-)}(N, l) + J_{2(+)}(N,l) + J_{2(-)}$$
(3.4)

$$J_{1(\pm)}(N, l) = \pm \int_{0}^{\infty} \frac{\Psi(q)}{2q} \sin N \left[q \pm \varphi(q) \right] \cos lq \, dq \tag{3.5}$$

$$J_{2(\pm)}(N,l) = \pm \int_{0}^{\pi} \frac{\Psi(q)}{2q} \cos N \left[q \pm \Psi(q) \right] \sin lq \, dq \tag{3.6}$$

Using the fact that $N \gg l$, we can apply the method of stationary phase [4,5] to the integrals (3.5) and (3.6). As a result of (3.2) the integrals $J_{1(-)}$ and $J_{2(-)}$ break down into asymptotic series in integral powers of the small quantity $N^{-1/3}$, where $J_{1(-)}$ is in even powers beginning with the zero power, and the integral $J_{2(-)}$ is in odd powers beginning with the first. The integrals $J_{1(+)}$ and $J_{2(+)}$ break down in integral powers of N^{-1} , the first in even powers beginning with zero, the second in odd powers beginning with one. Dropping terms of the expansions which approach zero faster than $N^{-1/3}$ as $N \to \infty$, we can write

$$J(N, l) \approx \psi(0) \left[\frac{1}{6} \pi - 0.703 | \varphi'''(0) | \frac{-1}{3} N \frac{-1}{3} \right], \quad \varphi'''(0) < 0$$

$$J(N, l) \approx \psi(0) \left[\frac{1}{3} \pi - 0.703 | \varphi'''(0) | \frac{-1}{3} N \frac{-1}{3} \right], \quad \varphi'''(0) > 0$$
(3.7)

Here we must differentiate the two cases $\varphi'''(0) < 0$ and $\varphi'''(0) > 0$. In the first case the approximate value of the integral $J_{1(-)}$ is negative, in the second case it is positive. Although the possibility of the existence of a positive third derivative of the function $\varphi(q)$ for q = 0 seems questionable (in this case the low-frequency vibrations have group velocities greater than the speed of sound) the present authors have not discovered any facts which forbid this possibility; therefore both cases are studied here.

In the new approximation the shock wave front is slanted, and in the course of time the slope decreases as $N^{-1/3}$. From (3.3) and (3.7) we can obtain the length of the slanted part of the shock wave front,

$$l_* \approx 2.2 |\varphi^{\prime\prime\prime}(0)|^{1/3} N^{1/3}$$

In the simple one-dimensional chain, if we take into account interaction only of the nearest neighbors, $\varphi^{m}(0) = -1/4$, in this case $l_* \approx 1.4 \text{ N}^{1/3}$. Thus, in the harmonic approximation of crystal-lattice dynamics the length of the slanted part of the shock wave front increases in the course of time; however, its relative length l_*/N diminishes in the course of time and tends to zero as $N \to \infty$. We note that if $\varphi^{m}(0) = 0$ the length of the slanted part of the shock wave front increases with time more slowly, namely as $N^{1/5}$. We can see from (3.7) that the distance traveled by the shock wave front $x_3 = \text{ct}$ is determined by the position of a point of the slanted part of the front, where in the case $\varphi^{m}(0) < 0$ the lattice compression reaches 1/3 (in the case $\varphi^{m}(0) > 0 - 2/3$) of the compression in the region located behind the shock wave front.

Significant corrections to the macroscopic approximation (3.3) of integral (3.1) are also the low-frequency vibrations, which propagate in the case $\varphi^{""}(0) \leq 0$ with velocities somewhat less than the speed of sound, and in the case $\varphi^{""}(0) \geq 0$ with speeds somewhat greater than the speed of sound. We can see from the asymptotic expansions presented in [2] that the amplitudes of these corrections increase with approach to the slanted part of the shock wave front. The stationary-phase method makes it possible to estimate at what distance l_{**} from the wave front the amplitudes of these corrections are Q times less than the amplitude of the step wave (3.3):

$$l_{**} \approx 0.9 \; (Q^4 N \,|\, \varphi^{\prime\prime\prime}(0) \,|)^{1/s}$$

if Q = 10 and $\varphi^{\text{III}}(0) = -1/4$, then $l_{**} \approx 13 \text{ N}^{1/3}$. If in this case N = 1000, then $l_{**} \approx 130$, if N = 10^8 , $l_{**} \approx 6000$. The quantity l_{**} increases in the course of time as N^{1/3}. However, the ratio of this quantity to the distance traveled by the wave front (l_{**}/N) diminishes and approaches zero as N $\rightarrow \infty$.

Also among the corrections to the macroscopic picture are the vibrational disturbances propagating with all possible velocities from the point of origin of the shock wave. Among these the disturbances associated with the inflection points of the dispersion curves damp most slowly (as $\tau^{-1/3}$). In the course of time the contribution of these corrections becomes very small.

From the physical viewpoint it is interesting to dwell on those cases in which the direction of collision is the axis of symmetry of the crystal. Here we can verify the Hugoniot relations [1]. The results obtained above make it possible to state that during collision of harmonic lattices (in contrast with anharmonic [6]) the Hugoniot relations are satisfied. In this case we discover a feature which is characteristic only of the harmonic approximation of lattice dynamics—the kinetic energy of the moving crystal is completely transformed into "elastic" compression energy and thermal vibrations of the atoms are not excited.

4. Crystal sublattice shifts. In studying various physical phenomena (the piezoeffect, for example) it is important to know how the Bravais lattices which comprise the complex lattice displace as a result of crystal deformation. Thus, bearing in mind (2.2), we can obtain from (2.1)

$$\kappa_{n\nu\lambda i}(t) = -\sum_{s, \mu} \frac{M\mu\nu}{M\pi} \left\{ \int_{0}^{\pi} \operatorname{Re}\left[e_{(s)\mu3}(q) \left(e_{(s)\nu i}\left(q\right) - e_{(s)\lambda i}\left(q\right) \right) \right] \times \frac{\sin\left[\omega_{(s)}(q) t\right]}{\omega_{(s)}(q) \sin^{1}/2 q} \sin\left(n + \frac{1}{2}\right) q d q + \frac{1}{2} \int_{0}^{\pi} \operatorname{Im}\left[e_{(s)\mu3}(q) \left(e_{(s)\nu i}\left(q\right) - e_{(s)\lambda i}\left(q\right) \right) \right] \frac{\sin\left[\omega_{(s)}\left(q\right) t\right]}{\omega_{(s)}(q) \sin^{1}/2 q} \cos\left(n + \frac{1}{2}\right) q d q \right\}$$
(4.1)

Taking into account (1.5) and (2.4), and the equality

$$\sum_{\mu} M_{\mu} e_{(s)\mu j} = 0, \qquad s = 4, 5, ..., 3 (p+1)$$

(see, for example, [7], p 75), we can see that undamped disturbances are contained only in the integrals of the lower line of (4.1) and only if s = 1, 2, 3. From (4.1) we identify three sublattice shift step waves

$$\kappa_{(s)\nu\lambda i}(t,n) = \begin{cases} -ave_{(s)3}(0) \left(e^{\circ}_{(s)\nu i} - e^{\circ}_{(s)\lambda i} \right) / c_{(s)}, & c_{(s)}t > na \\ 0, & c_{(s)}t < na \\ e^{\circ}_{(s)\nu i} = \lim_{q \to 0} \frac{1}{q} \operatorname{Im} e_{(s)\nu i}(q) \end{cases}$$
(4.2)

Comparing (4.2) and (2.5), we can write

$$\sigma_{(s)i} / \varkappa_{(s)v\lambda i} = e_{(s)i}(0) / a \left(e^{\circ}_{(s)vi} - e^{\circ}_{(s)\lambda i} \right)$$

$$(4.3)$$

Thus, in order to know how the crystal deformations and its sublattice shifts are interconnected we must find out how the quantities $e_{(s)i}(0)$ and $e^{\circ}_{(s)vi} - e^{\circ}_{(s)\lambda i}$ are interrelated.

In connection with the discussion above, we study the behavior of the acoustic branches of the spectrum as $q \rightarrow$ 0. Then

$$\lim_{q \to 0} \frac{\omega_{(s)}(q)}{q} = \frac{c_{(s)}}{a}, \quad \lim_{|\mathbf{k}| \to 0} \frac{\omega_{(s)}(\mathbf{k})}{|\mathbf{k}|} = c_{(s)}(\mathbf{k}_0), \quad \mathbf{k}_0 = \frac{\mathbf{k}}{|\mathbf{k}|}$$
(4.4)

In studying (1.4) as $q \rightarrow 0$ (in the general case as $|\mathbf{k}| \rightarrow 0$) it is more convenient to convert from the variables \mathbf{e}_{μ} to the variables

$$\mathbf{f}_{0} = \mathbf{e}_{0}, \quad \mathbf{f}_{\mu} = \mathbf{e}_{\mu} - \mathbf{e}_{0} \quad (\mu = 1, 2, ..., p)$$

$$\left\{ \sum_{\lambda=0}^{p} \mathbf{B}_{\nu\lambda}^{*}(\mathbf{k}) - M_{\nu}\omega^{2}(\mathbf{k}) \mathbf{E}^{*} \right\} \mathbf{f}_{0}(\mathbf{k}) + \sum_{\mu=1}^{p} \left\{ \mathbf{B}_{\nu\mu}^{*}(\mathbf{k}) - M_{\mu}\omega^{2}(\mathbf{k}) \,\delta_{\nu\mu} \mathbf{E}^{*} \right\} \mathbf{f}_{\mu}(\mathbf{k}) = 0$$

$$(4.5)$$

where ε^* is a third-order unit matrix; $e_{\mu}(\mathbf{k}) \equiv \{e_{\mu j}(\mathbf{k})\}$ are three-dimensional vectors, and $B_{\nu\mu}^*(\mathbf{k}) \equiv \{B_{\nu i\mu j}(\mathbf{k})\}$ are third-order matrices satisfying the relations

$$\sum_{\mu=0}^{p} B_{\nu i \mu j}(0) \equiv \sum_{\mathbf{m}, \mu} \Phi_{\mathbf{n} \nu i \mathbf{m} \mu j} = 0, \qquad \lim_{|\mathbf{k}| \to 0} \frac{1}{|\mathbf{k}|} \sum_{\nu, \mu=0}^{p} \operatorname{Im} B_{\nu i \mu j}(\mathbf{k}) = 0$$
(4.6)

The first identity (4.6) is well known, the second corresponds to the identities (23.11) of [8] and (59.5b) of [9] and can be obtained from them. Taking into account (4.4), the first identity (4.6), and letting $|\mathbf{k}| \rightarrow 0$ in (4.5), we obtain

$$\sum_{\mu=1}^{p} \mathbf{B}_{\nu\mu}^{*}(0) \, \mathbf{f}_{\mu}(0) = 0 \tag{4.7}$$

The matrix $B_{\nu i \mu j}$, $(\nu, \mu = 1, 2, ..., p)$, of order 3p, is nonsingular; otherwise the lattice would be unstable, namely sublattice shifts relative to one another without the action of external forces would be possible.

Thus, the 3p quantities $f_{\mu i}(0)$ ($\mu = 1, 2, ..., p$) equal zero, since they are solutions of a system of homogeneous linear equations whose matrix rank equals 3p.

We can see that the terms of (4.5) are zeros of different order with respect to $|\mathbf{k}|$ as $|\mathbf{k}| \rightarrow 0$, and the smallest order is unity. From (4.5) after dividing by $|\mathbf{k}|$ and passing to the limit $|\mathbf{k}| \rightarrow 0$ follows

$$\sum_{\mu=1}^{p} \mathbf{B}_{\nu\mu}^{*}(0) \, \mathbf{f}_{\mu}^{\circ} + \sum_{\lambda=0}^{p} \mathbf{B}_{\nu\lambda}^{\circ*} \, \mathbf{f}_{0}(0) = 0 \tag{4.8}$$
$$\mathbf{f}_{\mu}^{\circ} = \frac{1}{|\mathbf{k}|} \, \mathrm{Im} \, \mathbf{f}_{\mu}(\mathbf{k}), \qquad \mathbf{B}_{\nu\lambda}^{\circ*} = \lim_{|\mathbf{k}| \to 0} \frac{1}{|\mathbf{k}|} \, \mathrm{Im} \, \mathbf{B}_{\nu\lambda}^{*}(\mathbf{k})$$

As a result of the identities (4.6), of the 3(p+1) equations (4.8) with 3(p+1) unknowns only 3p will be linearly independent (for symmetry, let $\nu = 1, 2, ..., p$). The three equations which are lacking for completeness of the system can be obtained by summing (4.5) with respect to ν , dividing them by $|\mathbf{k}|^2$, and letting $|\mathbf{k}| \rightarrow 0$:

$$\{\mathbf{B}^* - Mc^2 \mathbf{e}^*\} \mathbf{f}_0(0) - \sum_{\lambda=1}^p \left(\sum_{\nu=0}^p \mathbf{B}_{\nu\lambda}^{\circ*}\right) \mathbf{f}_{\lambda}^{\circ} = 0$$
(4.9)

where

$$\mathbf{B}^* = \lim_{|\mathbf{k}| \to 0} \frac{1}{|\mathbf{k}|^2} \operatorname{Re} \sum_{\mathbf{v}, \ \lambda = 0}^p \mathbf{B}^*_{\mathbf{v}\lambda}(\mathbf{k}), \qquad M = \sum_{\mu = 0}^p M_{\mu}$$

Using the fact that the matrix of the left-hand side of (4.8) is nonsingular and solving the equations, we can obtain

$$\mathbf{f}_{\mu}^{*} = \mathbf{D}_{\mu}^{*} \mathbf{f}_{0}(0) \tag{4.10}$$

To clarify the complete picture of the sublattice displacements it is sufficient to examine only the displacements of all the sublattices relative to the basic sublattice. And these displacements, if we use (4.3) and (4.10), can be obtained from the crystal deformations

$$\varkappa_{(s)\nu 0} = D^*_{\nu} \sigma_{(s)}$$

It can be shown that in the case of a lattice, each atom of which is an inversion center, the sublattices shift so that the complex lattice as a whole undergoes only uniform deformation.

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