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A simple atomic model of a crack

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A CRACK in one-dimensional discrete medium is considered. The crystal is modelled by two infinite rows of atoms with an appropriate interaction between them. The forces of interaction between rows increase with distance in region I ($l \leqslant \lambda'$), decrease in region II ($\lambda' \leqslant l \leqslant \lambda$) and vanish in region III ($l > \lambda$), where λ and λ' denote some characteristic distances. In the rows, a nearest—neighbour interaction is assumed. Static solutions for a crack tip are given in analytic form and their dependence on external stress and physical parameters is discussed.

W pracy rozpatruje się szczelinę w jednowymiarowym ośrodku dyskretnym. Jako model kryształu przyjęto dwa rozciągające się do nieskończoności szeregi atomów, pomiędzy którymi istnieją odpowiednie oddziaływania. Siły oddziaływania między szeregami rosną z odległością w strefie I ($l \leqslant \lambda'$), maleją w strefie II ($\lambda' \leqslant l \leqslant \lambda$) i znikają w strefie III ($l > \lambda$), gdzie λ i λ' oznaczają pewne odległości charakterystyczne. W szeregach założono oddziaływanie najbliższych sąsiadów. W modelu tym otrzymuje się rozwiązania statyczne w formie analitycznej. W pracy zbadano rozwiązania dla końca szczeliny w zależności od naprężenia zewnętrznego i parametrów ośrodka.

В работе рассматривается щель в одномерной дискретной среде. Как модель кристалла приняты два, растягивающиеся в бесконечность, ряда атомов, между которыми существуют соответствующие взаимодействия. Силы взаимодействия между рядами возрастают с расстоянием в I зоне ($l \leqslant \lambda'$), убывают во II зоне ($\lambda' \leqslant l \leqslant \lambda$) и исчезают в III зоне ($l > \lambda$), где λ и λ' — некоторые характеристические расстояния. В рядах предположено взаимодействие самых близких соседей. В этой модели получаются статические решения в аналитической форме. В работе исследованы решения для конца щели в зависимости от внешнего напряжения и параметров среды.

1. Introduction

THE MAIN aim of this work consists in constructing a simple atomic model of a crack. The simplifications introduced are intended to allow a discussion of a crack (particularly a crack tip) in terms of exact analytic solutions. Instead of a three-dimensional crystal, we shall consider here a model consisting of two parallel infinite rows of atoms in xy-plane. The rows are extended in x-direction, while the atoms are allowed to move in y-direction. Within each of the rows, a non-central linear nearest-neighbour interaction is assumed. In addition, a simplified central non-linear interaction between the atoms of different rows is introduced. This is illustrated with Fig. 1, where the atoms and the corresponding interatomic bonds are represented by dots and "springs", respectively. The last interaction is assumed to disappear for sufficiently large distances between the interacting atoms. Within the range of non-vanishing interaction the row-row binding potential is approximated by two parabolic pieces. A similar simplification of a non-linear interaction turned out to be valuable in the case of Frenkel-Kontorova model of a dislocation, INDENBOM and ORLOV (1962), KRATOCHVIL and INDENBOM (1963), WEINER and SANDERS [(1964). A crack model involving non-linear interaction has been presented by J. N. GOODIER and M. KANNINEN (1968). In this model, however, the crystal is replaced by two continuous

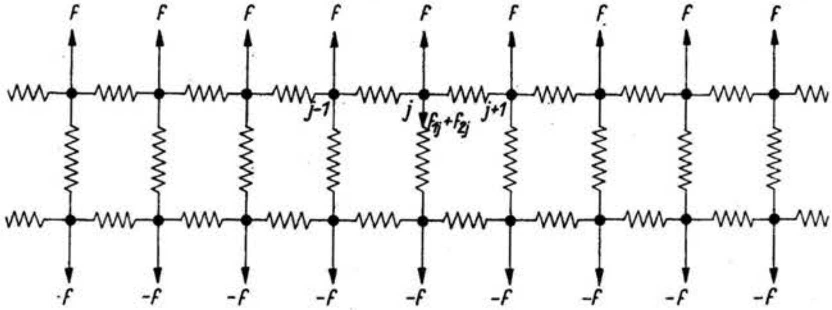

FIG. 1. Double-row model of an ideal crystal.

half-spaces. Thus the *GK* model is not "atomic": in dislocation terminology it corresponds rather to Peierls-Nabarro model.

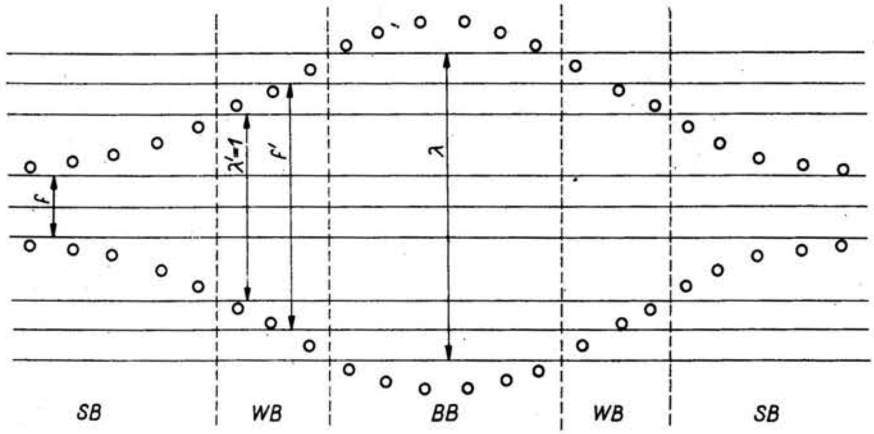

FIG. 2. A crack-type configurations of atoms.

We shall investigate the behaviour of the model under action of a uniform tensile stress $\sigma_{yy} > 0$. This stress is imitated by appropriate external forces acting upon the upper/lower row in positive/negative y-direction, respectively.

2. Equations of the model

Let us introduce the following notation (Fig. 1): f is the external force acting on each atom of the upper row; the corresponding force on the lower row equal $-f$; u_j—elongation of the j-th vertical bond; the corresponding displacements of the upper/lower atoms equal $\pm u_j/2$.

Because of the symmetry with respect to transformation $y \to -y$, it suffices to write equilibrium equation for one (the upper) row of atoms. It can be written as

$$f_{1j}+f_{2j} = f, \tag{2.1}$$

where f_{1j} denotes the force of the j-th vertical bond, f_{2j}—the force of the two succesive horizontal bonds on the j-th atom between them.

According to the assumption of a piece-wise parabolic potential of vertical bonds, the force f_1, as a function of bond extension u, is defined by the following equations:

$$f_1 = \begin{cases} au & \text{for} \quad u \leqslant \lambda', \\ a\lambda' \dfrac{\lambda - u}{\lambda - \lambda'} & \text{for} \quad \lambda' \leqslant u \leqslant \lambda, \\ 0 & \text{for} \quad \lambda \leqslant u, \end{cases} \tag{2.2}$$

where a, λ', λ are certain constants which characterize the strength and range of vertical interactions.

The plot $f_1(u)$ is shown in Fig. 3.

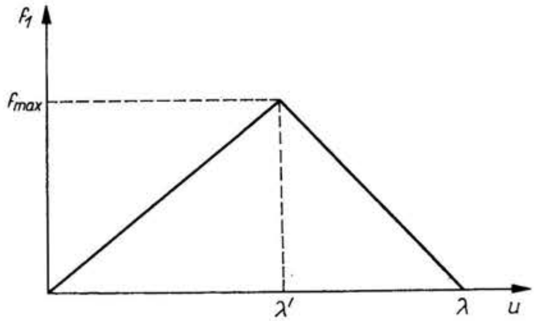

FIG. 3. Characteristics of a vertical bond.

Thus, depending on magnitude of u, three states of a vertical bond can be considered:

$$\begin{aligned} u &\leqslant \lambda' \text{ — a strong bond (SB)}, \\ \lambda' \leqslant u &\leqslant \lambda \text{ — a weak bond (WB)}, \\ \lambda &\leqslant u \text{ — a broken bond (BB)}. \end{aligned} \tag{2.3}$$

The maximal force which can be transmitted by a vertical bond equals

$$f_{\max} = a\lambda'. \tag{2.4}$$

From the definition of the force f_2, it follows that

$$f_{2j} = -(b/2)(u_{j+1} + u_{j-1} - 2u_j), \tag{2.5}$$

where the constant b characterizes the strength of horizontal bonds. The constant b is related to the shear modulus G in xy-plane, while the constant a—to the Young modulus E in y-direction.

On substituting Eq. (2.2) and (2.4) into Eq. (2.1), we obtain the following equations for strong, weak, and broken bonds, respectively:

$$\begin{aligned} au_j - (b/2)(u_{j+1} + u_{j-1} - 2u_j) &= f, \quad \text{(SB)} \\ \frac{a\lambda'}{\lambda - \lambda'}(\lambda - u_j) - (b/2)(u_{j+1} + u_{j-1} - 2u_j) &= f, \quad \text{(WB)} \\ -(b/2)(u_{j+1} + u_{j-1} - 2u_j) &= f. \quad \text{(BB)} \end{aligned} \tag{2.6}$$

Now, we are free to chose arbitrarily the units of length and force. Let these units be:

$$\lambda' = 1, \quad f_{\max} = 1. \tag{2.7}$$

The Eqs. (2.6) take the form

$$\begin{aligned} \nabla^2 u_j - P u_j + P f &= 0, \quad \text{(SB)} \\ \nabla^2 u_j + Q u_j - Q f' &= 0, \quad \text{(WB)} \\ \nabla^2 u_j + P f &= 0, \quad \text{(BB)} \end{aligned} \tag{2.8}$$

where ∇^2 denotes the second-order difference operator and

$$P = 2a/b, \quad Q = \frac{\lambda'}{\lambda - \lambda'} P = P/\lambda - 1, \tag{2.9}$$

$$f' = \lambda - (\lambda - 1) f. \tag{2.10}$$

As a set of independent non-dimensional quantities one can choose P, $\lambda = \frac{\lambda}{\lambda'}$ and $f = f/f_{\max}$. These quantities are restricted by the following inequalities

$$P > 0, \quad \lambda > 1, \quad 0 \leqslant f \leqslant 1. \tag{2.11}$$

In consequence,

$$1 \leqslant f' \leqslant \lambda. \tag{2.12}$$

3. General solutions

Any particular configuration u_j, according to the inequalities (2.3), determines a division of the chain into compact regions of strong, weak or broken bonds. Generally, several regions of the same type may be involved. Each of these regions is governed by an appropriate equation from the set (2.8). The general solutions for particular regions are given below.

1) SB—type region:

$$u_j^s = f + A\beta^{-j} + A'\beta^j, \tag{3.1}$$

where

$$\beta = (1/2)\left(2 + P - \sqrt{P^2 + 4P}\right) < 1 \tag{3.2}$$

and A, A' denote arbitrary constants.

2) WB—type region:

$$u_j^w = f' + B_1 \cos j\theta + B_2 \sin j\theta, \tag{3.3}$$

where

$$\cos\theta = 1 - Q/2 \tag{3.4}$$

and B_1, B_2 denote arbitrary constants.

In the case of $Q > 4$, the angle θ in the Eq. (3.4) must be complex. For the sake of definiteness, we shall take

$$0 < \theta < \pi \quad \text{for} \quad Q < 4 \tag{3.5}$$

and

$$\theta = \pi + i\theta', \quad 0 \leqslant \theta' < \infty \quad \text{for} \quad Q \geqslant 4. \tag{3.6}$$

3) BB—type region:

$$u_j^B = C + C'j - (Pf/2)j^2, \tag{3.7}$$

where C, C' denote arbitrary constants.

The arbitrary constants in all the regions involved are to be calculated from inter-region compatibility of solutions and boundary conditions at infinity.

An example of crack-type configuration is shown in Fig. 2. It involves five regions: SB, WB, BB, WB, SB. The regions of SB-type extend to infinity on both sides of the crack. The regions of BB and WB-type can be identified with an open crack and the crack tips, respectively.

The model allows more complicated crack-type configurations, too. In this paper, we shall discuss the tip region in more detail.

4. A Semi-infinite chain

Let us consider a semi-infinte chain in the configuration shown in Fig. 4. For the sake of convenience, the atoms are numbered with half-integers.

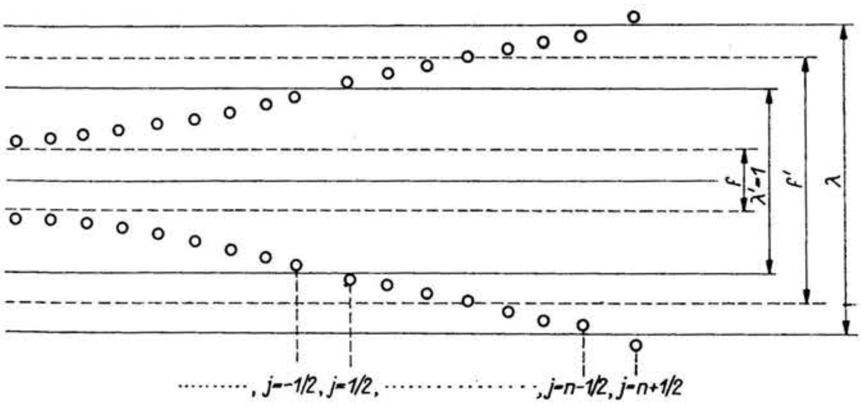

FIG. 4. Tip region of crack.

The configuration involves:

a SB-region from $j = -\infty$ to $j = -1/2$,

a WB-region containing n atoms from $j = 1/2$ to $j = n-1/2$,

a single atom $j = n+1/2$ with broken vertical bond (BB-type).

Thus

$$\begin{aligned} u_j &< 1 \quad \text{for} \quad j \leqslant -1/2, \\ 1 < u_j &< \lambda \quad \text{for} \quad 1/2 \leqslant j \leqslant n-1/2, \\ u_j &> \lambda \quad \text{for} \quad j = n+1/2. \end{aligned} \tag{4.1}$$

We shall discuss this configuration under the following assumptions:

1) the atoms $j \leqslant n-1/2$ are acted upon by the forces f,

2) the atom $j = n+1/2$ is acted upon by a given force F,

3) the displacements of the atoms in the WB-region depend on j monotonically:

$$u_{j-1} < u_j \quad \text{for} \quad 1/2 < j < n+1/2. \tag{4.2}$$

4) the solution u_j is bounded for $j \to -\infty$. Taking into account (3.1) and (3.3) and the boundary condition at infinity, we can write:

$$\begin{aligned} u_j &= u_j^s = f + A\beta^{-j} \quad \text{for} \quad j \leqslant 1/2; \\ u_j &= u_j^w = f' + \frac{B\cos j\theta}{2\cos\theta/2} + \frac{C\sin j\theta}{2\sin\theta/2} \\ &\qquad \text{for} \ -1/2 \leqslant j \leqslant n+1/2. \end{aligned} \tag{4.3}$$

From compatibility of u_j^s and u_j^w for $j = \pm 1/2$, we obtain the following equations for B and C:

$$\begin{aligned} B &= 2(f-f') + A(\beta^{1/2} + \beta^{-1/2}), \\ C &= A(\beta^{-1/2} - \beta^{1/2}). \end{aligned} \tag{4.4}$$

In the foregoing considerations, it will be important to introduce the force F_j transmitted by j-th horizontal bond. The horizontal bonds will be numbered by integer j's, the j-th bond connecting atoms labelled $j \pm 1/2$. The force F_j equals

$$F_j = (b/2)(u_{j+1/2} - u_{j-1/2}). \tag{4.5}$$

The boundary condition (2), which now takes the form

$$F_n = F, \tag{4.6}$$

enables us to express the unknown constant A by the force F.

In terms of F_j, the condition (3) can be expressed by inequalities

$$F_j > 0 \quad \text{for} \quad j = 0, \ldots, n. \tag{4.7}$$

From these inequalities a restriction of possible values of n follows. Taking into account (4.3), we obtain

$$n < \pi/\theta. \tag{4.8}$$

5. Transformation to new variables

A simplification of the discussion can be achieved by passing to some new variables. Instead of u_j and F_j we shall introduce ξ_j and Φ_j defined by the following equations:

$$\begin{aligned} u_j &= f'(1-f)\xi_j, \quad \text{half-integer } j\text{'s}. \\ F_j &= (b/2)(1-f)\Phi_j, \quad \text{integer } j\text{'s}. \end{aligned} \tag{5.1}$$

In the WB-region, the following equation is satisfied:

$$\nabla^2 \xi_j + Q\xi_j = 0, \quad -1/2 \leqslant j \leqslant n+1/2. \tag{5.2}$$

Next, instead of f and A, we shall use

(5.3) $$\xi = \frac{\lambda - f'}{1-f},$$

(5.4) $$K = \frac{A\beta^{-1/2}}{1-f}.$$

It follows from inequalities (2.11) and (2.12) that the admisible values of ξ are

(5.5) $$\infty > \xi \geqslant 0.$$

The solution expressed in terms of the new quantities reads

(5.6) $$\xi_j = K\{\sin(j+1/2)\theta\} - \lambda\frac{\cos j\theta}{\cos\theta/2}, \quad -1/2 \leqslant j \leqslant n+1/2,$$

where

(5.7) $$\{\sin k\theta\} \stackrel{\mathrm{df}}{=} \frac{1}{\sin\theta}\big(\sin k\theta - \beta\sin(k-1)\theta\big).$$

Similarly

(5.8) $$\Phi_j = K\{\cos j\theta\} + \lambda\frac{\sin\theta/2\sin j\theta}{\cos\theta/2},$$

where

(5.9) $$\{\cos j\theta\} = \frac{1}{\cos\theta/2}\big(\cos(j+1/2)\theta - \beta\cos(i-1/2)\theta\big), \quad 0 \leqslant j \leqslant n.$$

Under the restrictions (4.8), for the inequalities (4.1) and (4.7) to be satisfied, it is necessary and sufficient that the inequalities

(5.10) $$1 < K < \beta^{-1},$$

(5.11) $$\xi_{n-1/2} < \xi < \xi_{n+1/2}$$

be valid.

6. Admissible configurations

The problem of determining possible configurations of the semi-infinite chain can now be solved in the following way.

1. Consider ξ_j and Φ_j for the limiting values of K specified in (5.10), i.e., $K = 1$ and $K = \beta^{-1}$. From (5.6) and (5.8), we obtain the following identities:

(6.1) $$\xi_j(K = \beta^{-1}) = \xi_{j+1}(K = 1),$$

(6.2) $$\Phi_j(K = \beta^{-1}) = \Phi_{j+1}(K = 1).$$

Thus it is convenient to introduce the extended K-axis composed of segments $\{1 < K < \beta^{-1}, j\}$ corresponding to different values of j and such that the point $(K = \beta^{-1}, j)$ is identified with the point $(K = 1, j+1)$. Then the Eqs. (5.6) and (5.8) can be represented by piece-wise linear plots which, by the Eqs. (6.1) and (6.2), are continuous. The corresponding slopes are constant within each segment. Thus the plots of ξ_j and Φ_j are uniquely determined by the characteristic values

(6.3) $$\gamma_j \stackrel{\mathrm{df}}{=} \xi_j(K = \beta^{-1})$$

or

$$\psi_j \overset{\mathrm{df}}{=} \Phi_j(K = \beta^{-1}). \tag{6.4}$$

Moreover,

$$\psi_j = \gamma_{j+1/2} - \gamma_{j-1/2}. \tag{6.5}$$

2. The slopes of plots of ξ_j and Φ_j, according to (5.6) and (5.8), are given by the sine and cosine brackets (5.7) and (5.9). We shall briefly discuss these brackets.

Consider the root j_1 of the sine bracket (5.7),

$$\{\sin j_1\theta\} = 0, \quad 0 < j_1 < \pi/\theta. \tag{6.6}$$

It turns out that there is exactly one solution of (6.6) which satisfies the inequalities

$$(\pi/2\theta)+1/2 < j_1 < \pi/\theta. \tag{6.7}$$

The value of j_1 depends on β and θ. It decreases from π/θ to $(\pi/2\theta)+1/2$, if β increases from 0 to 1.

Let us define an integer number n_1 by the inequalities

$$n_1 \leqslant j_1 < n_1+1. \tag{6.8}$$

For $j = n_1$, we have

$$\{\sin n_1\theta\} \geqslant 0. \tag{6.9}$$

Thus the slope of the broken line representing ξ_j is positive (or equal to zero) for $j \leqslant n_1-1/2$ and negative for $j \geqslant n_1+1/2$.

Similarly, there exists exactly one root j_0 of the cosine bracket (5.9):

$$\{\cos j_0\theta\} = 0, \quad 0 < j_0 < \frac{\pi}{\theta}. \tag{6.10}$$

It satisfies the inequalities

$$0 < j_0 < (\pi/2\theta)-1/2. \tag{6.11}$$

The value of j_0 increases from 0 to $(\pi/2\theta)-1/2$, if β decreases from 1 to 0. We shall define an integer n_0 by the inequalities

$$n_0 \leqslant j_0 < n_0+1. \tag{6.12}$$

We have

$$\{\cos n_0\theta\} \geqslant 0. \tag{6.13}$$

Hence, the slope of the broken line representing Φ_j is positive (or equal to zero) for $j \leqslant n_0$ and negative for $j \geqslant n_0+1$. The integers n_0, n_1 satisfy the inequality

$$n_0 \leqslant n_1-1 \tag{6.14}$$

for arbitrary values of θ and β. For given θ and β, the values of n_0, n_1 can be determined from Fig. 5.

3. Making use of equations (5.2), (5.6), (5.8) and (6.5), we arrive at the following identity:

$$-\{\cos j\theta\} = \frac{4\beta\sin^2\theta/2\cos\theta/2}{1-\beta}\gamma_{j-1/2}. \tag{6.15}$$

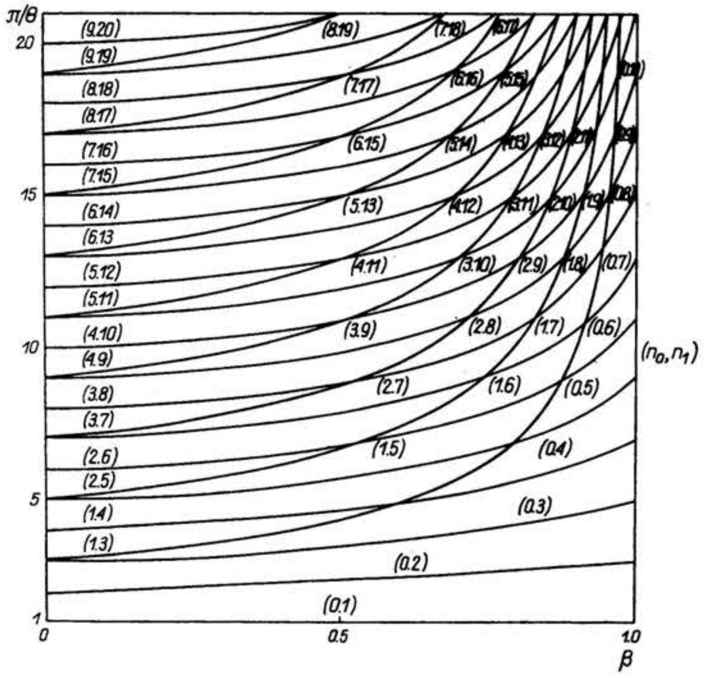

FIG. 5. The integers (n_0, n_1) as functions of θ, β.

It shows that

$$(6.16) \qquad \gamma_j < 0 \quad \text{for} \quad j = n_0 - 1/2,$$
$$\gamma_j > 0 \quad \text{for} \quad j \geqslant n_0 + 1/2.$$

Thus we can conclude that the broken line $\xi_{n+1/2}$ intersects the extended K-axis in the segment $\{K, n_0\}$. Similarly, from (6.5), we conclude that the broken line Φ_n intersects the extended K-axis in the segment $\{K, n_1\}$. The general shape of the plots of $\xi_{n+1/2}$ and Φ_n is shown in Fig. 6.

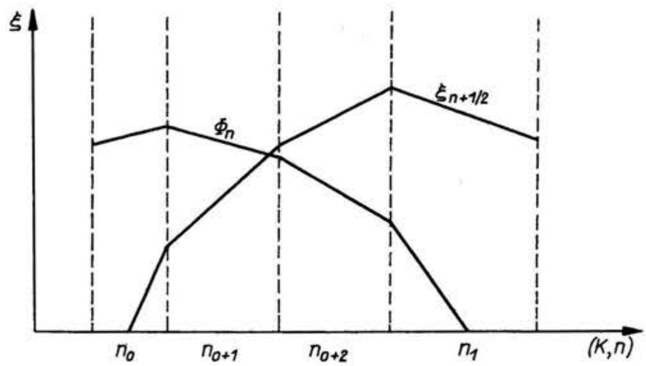

FIG. 6. The plots of $\xi_{n+1/2}$ and Φ_n.

7. The solutions

Now, we shall pass to the (ξ, Φ)-plane, with Φ defined as

$$\Phi = \frac{P}{1-f}F. \tag{7.1}$$

The condition (4.6) reads

$$\Phi_n = \Phi. \tag{7.2}$$

From the shape of the plot of Φ_n it is evident that there exists an upper limit $\Phi_{\max}$ for Φ:

$$\Phi < \Phi_{\max} = \psi_{n_0} = \beta^{-1}\{\cos n_0\theta\} + \lambda \tan\theta/2 \cdot \sin n_0\theta. \tag{7.3}$$

Thus, for some values of Φ, two solutions will exist. Therefore we introduce the extended Φ-axis composed of two pieces: from 0 up to $\Phi_{\max}$ and then from $\Phi_{\max}$ down.

In order to determine the solutions, we shall draw the limiting values from (5.11) in the extended (ξ, Φ)-plane. The plot of $\xi_{n-1/2}$ can be obtained from that of $\xi_{n+1/2}$ by shifting the latter by one segment along the extended K-axis. After transforming the relevant plots to the extended (ξ, Φ)-plane, we obtain the plots which, for some particular values of θ and β, are shown in Fig. 7 and Fig. 8. The region of admissible solutions lies between the curves $\xi_{n-1/2}$ and $\xi_{n+1/2}$. Any particular solution is represented by the point of intersection of the straight lines corresponding to given values of ξ and Φ (i.e. f and F). The values of ξ and Φ are compatible with each other if, and only if, the corresponding point of intersection lies in the admissible region.

For such ξ, Φ, a solution always exists. It is necessary to remember that any value of Φ is represented by two points of the extended Φ-axis and both the vertical lines must be

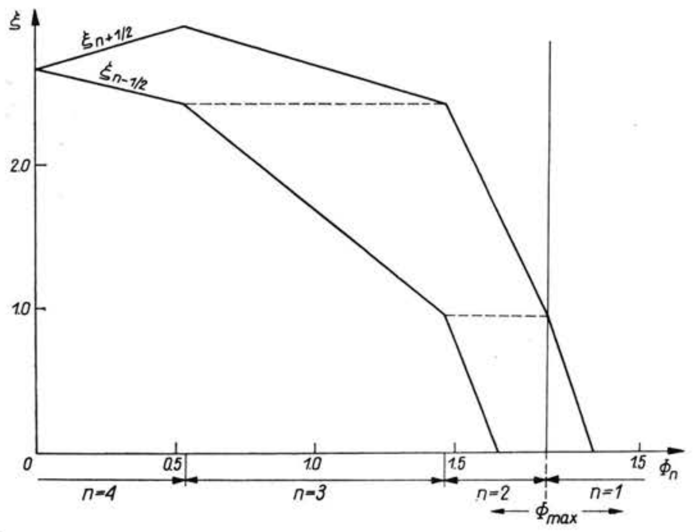

FIG. 7. The region of admissible solutions for $\beta = 0.4$, $\pi/\theta = 5$, $(n_0 = 1,\ n_1 = 4)$.

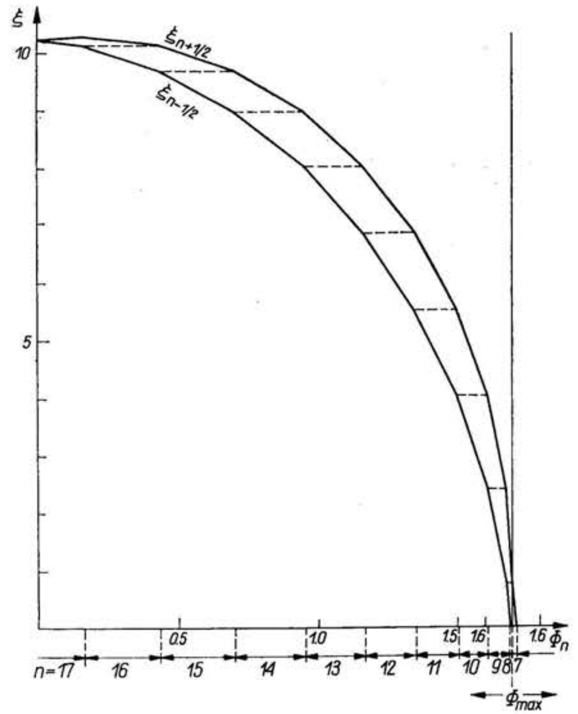

FIG. 8. The region of admissible solutions for $\beta = 0.6$, $\pi/\theta = 19$, ($n_0 = 7$, $n_1 = 17$).

drawn. If the points of intersection with the horizontal ξ-line both belong to the admissible region, then two solutions exist. In that case, they will correspond to $n = n_0$ and $n = n_0+1$.

Generally, n_0 is the smallest admissible value of n (i.e. the number of weak bonds in the tip region). It is achieved if the force F approaches its maximal value. On the other hand, n_1 represents the largest possible value of n. The number of weak bonds equals n_1, if the force F approaches 0.

In the case of $F = 0$, the only admissible value of ξ is represented by the point of intersection of the $\xi_{n+1/2}$ and $\xi_{n-1/2}$ lines:

$$\xi_{cr} = \frac{-\gamma_{n_1+1/2}\gamma_{n_1-3/2}+\gamma^2_{n_1-1/2}}{4\sin^2\theta/2\cdot\gamma_{n_1-1/2}}, \tag{7.4}$$

and is always positive.

If $Q > 4$ (i.e. θ is a complex number), the only possible values of n are 0 and 1. For θ decreasing towards zero, the numbers n_0, n_1 and the difference $n_1 - n_0$ increase.

The maximum value of ξ for which a solution may exist equals

$$\xi_{max} = \gamma_{n_1-1/2} = \beta^{-1}\{\sin n_1\theta\} - \lambda\frac{\cos(n_1-1/2)\theta}{\cos\theta/2} > \xi_{cr}. \tag{7.5}$$

For any given $\xi < \xi_{max}$, two succesive values of n are only allowed.

References

1. V. L. INDENBOM and A. N. ORLOV, Usp. Phys. Nauk, **76**, 557, 1962.
2. J. KRATOCHVIL and V. L. INDENBOM, Czech. J. Phys., **13**, 814, 1963.
3. J. H. WEINER and W. T. SANDERS, Phys. Rev., **134**, A1007, 1964.
4. "Fracture", Volume 2, edited by H. LIEBOWITZ, 43–50, 1968.

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