The tensile load on a polymer chain extending across an amorphous region of an amorphous-crystalline polymer, from one crystal to another, has been calculated theoretically. The analysis is carried out for the case of large extensions of the amorphous region, when it is necessary to take into account the conditions of anchorage of the chain at the external boundaries of the crystals. A rigorous criterion has been established for the applicability of an earlier theory [1] in which the external boundaries were not taken into consideration. It is concluded that the critical load on the chains cannot be reached in that model in the range of deformations of the amorphous region studied. It is noted that the expression for the displacement of the chain segments is a solution of the Frenkel-Kontorov model of a point dislocation in a crystal with a boundary.

The mechanics of a macromolecule bridging an amorphous region between two crystals were studied in [1]. However, in that paper the external boundaries of the crystals were not taken into account. A rough appraisal of the validity of the model showed that in the case of kapron (nylon-6) the theory holds when \( \rho \) is less than half the length of one monomer unit. Here \( \rho \) (see [1]) represents the length of the part of an unstretched chain pulled out by an external load into the amorphous region.

In order to investigate the dependence of chain tension, on the length of the amorphous region at large extensions of the amorphous region (i.e., at high values of \( \rho \)) we will construct an analogous theory, taking into account the external crystal boundaries. This will also enable the limits of applicability of the theory of [1] to be rigorously formulated.

It should be noted in passing that the equations derived below for the displacement of chain elements are in fact a solution to the Frenkel-Kontorov model of a point dislocation in a crystal with a boundary. They could be useful, for instance, in the study of the problem of stacking faults [2].

**Basic equations of the theory and their solution.**

The model of [1] is adopted, the only difference being that the crystalline regions are now considered to be finite. The equilibrium equation of the chain within the crystal (see [1], Eq. (4)) is

\[
\frac{d^2 u}{d\lambda^2} = 2\alpha \sin 2\pi u.
\]  

(1)

The notation is as in [1]; the only difference is that all quantities having the dimension of length (i.e., \( u, y, \rho, b, L \)) are here considered to be dimensionless, expressed in monomer unit lengths. The first integral of Eq. (1) is

\[
\left( \frac{du}{dy} \right)^2 = \frac{\xi^2}{\tau} \left( A - \frac{1}{2} \cos 2\pi u \right),
\]  

(2)

where \( A \) is an integration constant which, by contrast with [1], cannot be taken as being equal to 1/2. Transforming the cosine, we get

\[
\left( \frac{du}{dy} \right)^2 = \frac{\xi^2}{\tau} \left( \frac{m_1}{m} + \sin^2 \pi u \right),
\]  

(3)

where \( m_1 = 1 - m \). Here \( m \) is a redefined constant of integration. Substituting

\[
t = \sin \pi u, \quad \tau = \frac{\pi \xi}{m}(y - \rho),
\]  

(4)

Eq. (3) can be reduced to

\[
\left( \frac{dt}{d\tau} \right)^2 = (1 - \xi^2)(m_1 + m\xi^2),
\]  

(5)

Its solution has the form (see [3, 4])

\[
t = \pm c n(\tau - B/m);
\]  

(6)

Fig. 1. Diagram showing the packing of the chains and their anchorage at the external boundaries of crystalline regions.

Fig. 2. Comparison of the interpolation equation (24) with the exact roots of Eq. (15). The solid lines are values of \( m_1 \) determined from the interpolation equation. The points are exact roots. The curve C is for old and H for new values of the parameters.
sn(τ/m), cn(τ/m) and du(τ/m) are Jacobian elliptic functions with argument τ and parameter m; B is the second constant of integration.

Fig. 3. Dependence of chain tension on ρ for old (curve C) and new (curve H) parameters.

Let us confine ourselves to the right-hand crystal in Fig. 1. Here, when the chain is pulled out from the crystal, u < 0; therefore

\[ u(ρ) = -\frac{1}{π} \arcsin cn \left[ \frac{πx}{y}(ρ-ρ) - B/m \right] \]  

(7)

The boundary condition at the internal boundary of the crystal is identical with that for a semi-infinite crystal (see [1], Eq. (8)):

\[ u(ρ) = -ρ. \]  

(8)

We reckon ρ from a point lying at the intersection of the chain with the interregional boundary in the absence of stress. We now formulate the boundary conditions at the external boundary of the crystal.

Crystalline regions of a polymer are made up of macromolecules whose length is considerably greater than the length r of the crystalline region. At the boundary of the crystal the macromolecule makes a turn and is again folded inside the crystal (see Fig. 1). But

\[ u(r) = 0. \]  

(9)

Conditions (6) and (9) in combination with (7) give

\[ cn(ρ/m) = \sin πp, \quad cn \left[ \frac{πx}{y}(r-ρ) - B/m \right] = 0. \]  

(10)

To determine the sign of B, we consider the limiting case of a semi-infinite crystal. Comparing Eq. (3) of this paper with Eq. (6) of [1], we may conclude that the semi-infinite model is a particular case of the present theory, corresponding to m = 1. It is apparent from physical considerations that as p decreases so does the effect of the external boundary of the crystal on the solution. We conclude from this that as p → 0 the solutions for chain displacements based on [1] and on the present model will tend toward each other, i.e., m → 1 as p → 0. However, as m → 1

\[ \lim_{m \to 1} \frac{πx}{y}(y-ρ) - B/m \to \sinh \left[ \frac{πx}{y}(y-ρ) - B \right]. \]  

(11)

Here and in Eq. (15) we have used the notation of Glaisher [3], p. 378. Combining Eqs. (7) and (11), we get a quadratic equation and determine \( e - \frac{πx}{y}(1 + ρ) \). Selecting a solution which corresponds to decrease of |u| with increasing y, we get

\[ e - \frac{πx}{y}(1 + ρ) = c e - \frac{πx}{y}(1 - ρ). \]  

(12)