

S.C., 0.24; it will thus be seen that for one lattice at least,  $p_c$  differs substantially from (1) to (2).

We have used the terminology "site mixtures" and "bond mixtures" to distinguish between the above two problems. The above series (1) and (2) have been derived by applying the standard techniques of the theory of cooperative phenomena in crystals<sup>7</sup> to these problems. The configurational problems involved contain new features but we have been able to employ special devices to extend the series. In this work we have been greatly helped by our colleagues M. E. Fisher and J. Essam, who have also independently

<sup>7</sup> C. Domb, *Advances in Physics*, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1960), Vol. 9, pp. 149-361.

derived closed-form approximations for the various quantities which enter.<sup>8</sup>

The methods have also been applied to nonideal mixtures in which the energies of interaction between  $A$  and  $B$  molecules are nonzero, and the variation of cluster size with temperature has been investigated. Details of the work referred to in this note are being published elsewhere.

#### ACKNOWLEDGMENTS

We are grateful to Dr. R. J. Elliott and Professor G. S. Rushbrooke and their collaborators for communicating details of their results to us.

<sup>8</sup> J. Essam and M. E. Fisher, *J. Math. Phys.* (to be published).

## Lorentz Force on Screw Dislocations and Related Problems

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The concept of a Lorentz force on screw dislocations, first introduced by Nabarro, is analyzed. It is concluded that the Nabarro-Lorentz force on screws and the Lorentz force of electromagnetism are not analogous, and that the term a Lorentz force on screws should be dropped in order to avoid confusion. Only when the screw is constrained to move on one slip plane is the analogy with electromagnetism complete. Total quasimomentum is not generally conserved when screw dislocations interact with elastic waves.

### INTRODUCTION

IN 1951 Nabarro<sup>1</sup> introduced the concept of a Lorentz force on screw dislocations, and since then this concept has been in current use and seems to be generally accepted. However, the published explanations of Nabarro<sup>1</sup> and Eshelby<sup>2</sup> do not unequivocally establish the existence of a true Lorentz force on screw dislocations.

Hence, the aim of the present paper is mainly pedagogical: We want to make unequivocal and easily understood statements about the forces on screw dislocations to clear away possible confusion. This paper should not be looked upon as a direct criticism of previous work. We merely want to emphasize that what has been termed the Lorentz force on screw dislocations is not in fact analogous to the Lorentz force in electromagnetism, and that consequently the term "a Lorentz force on screws" should be dropped in order to avoid confusion.

So far the Lorentz force on screws has been of little practical importance. It has been used in discussions on

dislocation mobility,<sup>1,3</sup> but these discussions do not really depend on the existence of a Lorentz force as the results obtained are used to illustrate the quasimomentum balance for elastic waves and screws constrained to move on *one* slip plane, in which case the electromagnetic analogy is complete. However, presently a great deal of interest is being directed towards high-velocity dislocations resulting from shock-loading, and in this field a possible Lorentz force would be important, according to Weertman.<sup>4</sup> Thus we should think that the concept of a Lorentz force on screws merits some discussion at the present time.

### DISCUSSION OF THE NABARRO-ESHELBY DERIVATION OF THE LORENTZ FORCE ON SCREWS

Eshelby<sup>2</sup> has given a simple derivation of the Nabarro-Lorentz force on screws, which is not essentially different from Nabarro's original derivation. Consider a procession of screws,  $n$  per unit length, oriented parallel to the  $z$  axis and with Burgers vector  $+b$  traveling across a bar of square cross section with a velocity  $v_x$  (Fig. 1). Then the upper part of the bar, I, will have a

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<sup>1</sup> F. R. N. Nabarro, *Proc. Roy. Soc. (London)* **A209**, 278 (1951).

<sup>2</sup> J. D. Eshelby, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1956), Vol. 3, p. 134.

<sup>3</sup> J. Lothe, *Phys. Rev.* **117**, 704 (1960).

<sup>4</sup> J. Weertman in *Response of Metals to High-Velocity Deformation* (Interscience Publishers, Inc., New York, 1961, to be published).

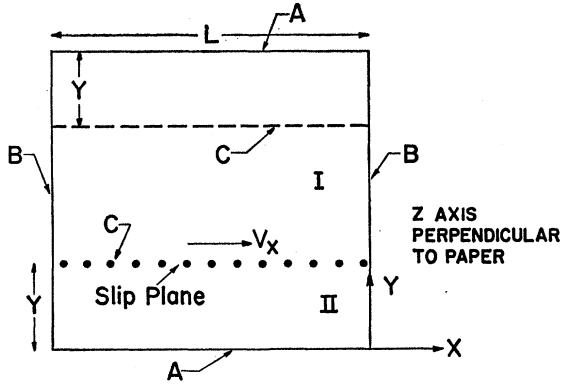


FIG. 1. Cross-section view of a bar traversed by a procession of screws.

velocity

$$V = -nbv_x, \quad (1)$$

in the  $z$  direction relative to part II. The average between the  $z$ -direction velocities on the two sides of the slip plane is termed  $\dot{u}$ . If the height of the procession is raised by  $\delta y$ ,  $V$  and  $\dot{u}$  being kept constant, the kinetic energy per unit depth of the crystal increases by an amount

$$\delta E_{\text{kin}} = nL\rho b v_x \dot{u} \delta y, \quad (2)$$

where  $L$  is the width of the cross section and  $\rho$  the density of material. This kinetic energy increment must be supplied by external forces doing work on the surface of the crystal. In accordance with the general definition of forces on dislocations in terms of derivatives of external work done when the dislocations move, it may be said that there is a force per unit length,

$$F_y = -\rho b v_x \dot{u}, \quad (3)$$

on each dislocation, resisting motion in the  $+y$  direction.  $F_y$  is the so-called Nabarro-Lorentz force, perpendicular to the direction of dislocation motion.

A shear stress exerts a force on a screw dislocation *and makes it move*. The arbitrary average velocity of the material along the dislocation,  $\dot{u}$ , has no importance for the dislocation motion relative to the crystal. Thus, the screws are not affected by the forces defined by Eq. (3), but are only influenced by the shear stresses.

In mechanics, a particle, moving in the  $x$  direction, will continue to do so if the total force on the particle has no  $y$  and  $z$  components. If we want the situation to be analogous for screw dislocations, the Nabarro-Lorentz force must be dropped because it cannot balance shear stress forces.

We should also point out that if a true Lorentz-type force acted on the screw, it could not be derived from an energy expression, since by definition Lorentz-type forces do no work and do not enter the energy expressions. Thus the energy change in Eq. (2) does not at all imply Lorentz-type forces on the screws. To make this point completely clear, we shall show how the energy

change Eq. (2) can be calculated under the assumption that screws are made to move by shear stresses *only*.

Suppose, that by applying pure shear stresses to the walls  $A$  and  $B$  we raise the dislocation wall upwards by  $\delta y$ , without any change in the resultant slip velocity  $V$ . Since, by hypothesis, only shear forces are employed, there can be no change in the total momentum per unit depth,

$$M = \rho L^2 \dot{u} - \rho y L V. \quad (4)$$

Under the condition that no changes in  $M$  and  $V$  occur, the change in kinetic energy per unit depth is found to be

$$\delta E_{\text{kin}} = (\frac{1}{2} \rho L V^2 - \rho y V^2) \delta y, \quad (5)$$

and, by Eq. (4), there is also a change in  $\dot{u}$ ,

$$\delta \dot{u} = V \delta y / L. \quad (6)$$

We next restore  $\dot{u}$  to its previous value by imparting a momentum  $\delta M = -\rho L V \delta y$  per unit depth to the bar, and, as the bar as a whole has a velocity  $\dot{u}$ , we then do an amount of work

$$\delta W = -\rho L V \dot{u} \delta y, \quad (7)$$

per unit depth.

Suppose this momentum  $\delta M$  is imparted to the bar by equal forces on the surfaces  $A$ . Shear stresses will then arise, which must be balanced out by an opposite external shear stress such that the screws are not accelerated. The central slab defined by the planes  $C$  (Fig. 1) has a thickness  $L - 2y$  and will be given a momentum  $-\rho(L - 2y)V\delta y$  per unit depth. Thus, if a time  $t$  is used to impart the momentum, the average shear stresses on the planes  $C$  will be of the magnitude

$$\delta \sigma = -\frac{1}{2Lt} \rho (L - 2y) V \delta y. \quad (8)$$

Thus, the work done on the dislocations by the external shear stress that we apply to balance out the shear stress Eq. (8) is

$$\delta \sigma L V t = (-\frac{1}{2} \rho L V^2 + \rho y V^2) \delta y. \quad (9)$$

Adding the expressions Eq. (5), Eq. (7), and Eq. (9) and using Eq. (1), we again obtain Eq. (2).

It is noted that the term Eq. (7) gives the contribution from which the Nabarro-Lorentz force is derived, and this is the only term which is not directly connected with dislocation motion. Therefore, as in the first example, it has been demonstrated that the concept of a Lorentz force is specious.

#### QUASIMOMENTUM CONSIDERATIONS FOR SCREWS

In electrodynamics two possible ways of deriving the Lorentz force exist when all the other Maxwell equations are given: (1) Postulate relativistic invariance, and (2) postulate conservation of the sum of particle and field momentum. The second method is suggestive of a

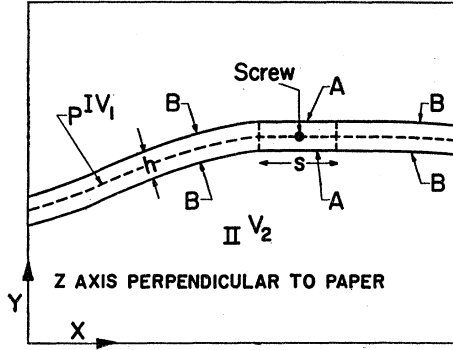


FIG. 2. Cross-sectional view of a bar traversed by a screw along the trajectory  $P$ . The trajectory is in the middle of a thin sheet of thickness  $h$ .  $A$  refers to the surface of a slab of width  $s$  symmetrical about the screw,  $B$  refers to the surface of the rest of the sheet.

theory for screws that will be illuminating for this discussion: We will directly employ the energy-momentum tensor of homogenous media to discuss quasimomentum (field-momentum) relations for the screw. As dislocation "momentum" is of the same kind as quasimomentum (field momentum), a Lorentz-type force on screws would imply that quasimomentum is conserved in the interaction between a screw and an elastic field.

Consider a homogeneous medium, and imagine that the medium can only be given displacements  $u$  in the  $z$  direction, and that the displacements do not depend on the  $z$  coordinate. In this two-dimensional case we have the conservation law,

$$\text{div} \tilde{T} = \partial g / \partial t. \quad (10)$$

$\text{div} \tilde{T}$  is defined as  $\mathbf{i} \text{div} \mathbf{T}_x + \mathbf{j} \text{div} \mathbf{T}_y$ , where  $\mathbf{T}_x = \mathbf{i} T_{xx} + \mathbf{j} T_{xy}$ , and  $\mathbf{T}_y = \mathbf{i} T_{xy} + \mathbf{j} T_{yy}$ .

Here

$$\mathbf{g} = -\rho \dot{u} \text{grad} u \quad (11)$$

is called the quasimomentum density. The expressions for the tensor components of  $\tilde{T}$  are

$$\begin{aligned} T_{xx} &= W - \sigma_{zx} \partial u / \partial x - \frac{1}{2} \rho \dot{u}^2, \\ T_{yy} &= W - \sigma_{zy} \partial u / \partial y - \frac{1}{2} \rho \dot{u}^2, \\ T_{xy} &= -\sigma_{zx} \partial u / \partial y, \\ T_{yx} &= -\sigma_{zy} \partial u / \partial x, \end{aligned} \quad (12)$$

where  $W$  is the strain energy density and  $\sigma_{zx}$  and  $\sigma_{zy}$  are the ordinary stress tensors.

For an explanation of the above formulas we refer to Eshelby.<sup>2</sup> It should be noted that only in the approximation of linear elasticity is  $T_{xy} = T_{yx}$ .

Now consider a crystal containing a screw, of vector  $\langle 0, 0, b \rangle$ , and consider the screw to be passing through the crystal along the path  $P$  (Fig. 2). For convenience, consider the screw when it is moving in the  $x$  direction. Then divide the crystal into two half-crystals I and II separated by a thin sheet of material of thickness  $h$ , in the middle of which the screw is moving. Divide out of

the sheet one small rectangular slab of width  $s$  symmetrical about the screw, with surfaces  $A$ .  $B$  is the surface of the rest of the sheet.

We consider the sheet to be so thin that stress, strain, and velocity is continuous from one half-crystal to the other across the sheet in the regions  $B$ . Across  $A$  we consider strain  $\partial u / \partial y$ , strain energy  $W$  and shear stress  $\sigma_{zy}$  to be continuous, while  $\partial u / \partial x$  change sign but has the same magnitude on the two sides.  $\partial u / \partial x$  is symmetric about a line parallel to the  $y$  axis and passing through the dislocation, while  $\sigma_{zy}$  is antisymmetric.

We postulate the above conditions always to be satisfied on the surface of the sheet of thickness  $h$ , which is defined by the screw trajectory. The screw dislocation is characterized by being unable to sustain an external shear stress. If we apply an external shear stress, the screw is postulated to move with such an acceleration and in such a direction that the above conditions are satisfied. The effective "mass" of the screw will depend roughly logarithmically on  $h$ , which will be of the order of magnitude  $b$  (one lattice distance). The inertial reaction of the material within the sheet is completely neglected. This is about the same approximation as employed previously by Eshelby<sup>5</sup> in treating the dynamic behavior of the screw. These assumptions should be representative of the general screw. A more detailed theory would have to consider the actual core structure, which would be different for different materials and crystal structures.

Now, integrating Eq. (10) over the volumes  $V_1$  and  $V_2$  and adding (we always consider the volume of unit depth), we obtain

$$\int_S \tilde{T} dS + \int_A \tilde{T} dS = \frac{d}{dt} \mathbf{G}, \quad (13)$$

where

$$\mathbf{G} = \int_V \mathbf{g} dV. \quad (14)$$

$S$  is the external surface of both half-crystals considered as one, and  $V$  is the total volume  $V = V_1 + V_2$ . The surface integrals over  $B$  cancel.

It is readily found that  $\int_A \mathbf{T}_x dS$  vanishes, so that

$$\int_S \mathbf{T}_x dS = \frac{d}{dt} \mathbf{G}_x. \quad (15)$$

For  $\mathbf{T}_y$  only the term  $-\frac{1}{2} \rho \dot{u}^2$ , Eq. (12), gives a net contribution to the integral over  $A$ . On the upper surface, the average velocity is  $\dot{u} - bv_x/2s$  so that

$$-\frac{1}{2} \rho (\dot{u} - bv_x/2s)^2 = -\frac{1}{2} \rho \dot{u}^2 + \rho b \dot{u} v_x / 2s - \frac{1}{8} \rho b^2 v_x^2 / s^2,$$

and similarly on the lower surface

$$-\frac{1}{2} \rho (\dot{u} + bv_x/2s)^2 = -\frac{1}{2} \rho \dot{u}^2 - \rho b \dot{u} v_x / 2s - \frac{1}{8} \rho b^2 v_x^2 / s^2.$$

<sup>5</sup> J. D. Eshelby, Phys. Rev. **90**, 248 (1953).

Only the middle terms on the right-hand sides of the above expressions contribute to the integral, so the final result is

$$\int_S \mathbf{T}_y d\mathbf{S} - \rho b \dot{u} v_x = \frac{d}{dt} G_y. \quad (16)$$

Suppose that the crystal is at rest and that the dislocation is locked. Then an external force

$$F_x = -b\sigma_{zy} = \int_S \mathbf{T}_x d\mathbf{S}, \quad (17)$$

acts on the screw. Suppose there is no  $F_y$  component. When the dislocation is unlocked, it will accelerate along a straight path parallel to the  $x$  axis in accordance with the equation

$$F_x = dG_x/dt. \quad (18)$$

Before the dislocation motion affects the surface of the specimen,  $dG_x/dt$  does not depend on an arbitrary velocity of the crystal as a whole, so apart from an arbitrary constant it is then unambiguous to call  $G_x$  the momentum of the dislocation in its direction of motion. The dislocation momentum is then of the same kind as the "momentum" of elastic waves.<sup>1</sup>

Next suppose the dislocation has been put into rectilinear motion along the  $x$  axis, and consider it *only before the dislocation motion reaches the surface*, which is considered to be at rest. Suppose that no external forces are present,  $\int_S \mathbf{T}_x d\mathbf{S} = \int_S \mathbf{T}_y d\mathbf{S} = 0$ . Then the dislocation will slow down as its mass increases.<sup>5</sup> The quantity  $G_x$  is conserved. The dislocation shows no tendency to move in the  $y$  direction. Nevertheless, if we ascribe an arbitrary uniform velocity  $\dot{u}$  to the crystal as a whole, the quantity  $G_y$  is *not conserved*, although no quasimomentum is pumped in at the external surface because

$$\int_S \frac{1}{2} \rho \dot{u}^2 d\mathbf{S} = \frac{1}{2} \rho \dot{u}^2 \int_S d\mathbf{S} = 0.$$

By Eq. (16) we simply obtain

$$-\rho b \dot{u} v_x = dG_y/dt. \quad (19)$$

So, in a crystal containing screws able to move in all directions, and with no quasimomentum being created at the external surface, total quasimomentum is not generally conserved.

It is instructive to apply the above results to a screw interacting with an elastic wave.

Consider a screw at rest at the origin, and a plane shear wave impinging upon it in the  $y$  direction (Fig. 3).

The incident shear wave makes the screw vibrate in the  $x$  direction, and elastic waves are scattered. The elastic wave possesses a  $y$  component of quasimomentum  $w/c$  per unit volume,  $w$  being the energy density and  $c$  the sound velocity. Let  $\sigma_{zy}$  be the shear stress in the impinging wave and  $v_x$  the dislocation velocity. Then an

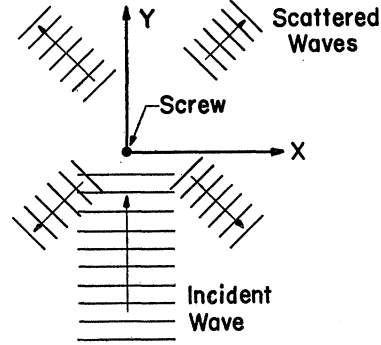


FIG. 3. A screw at the origin made to vibrate by an incident shear wave.

energy

$$-b\langle\sigma_{zy}v_x\rangle_{av} \quad (20)$$

is scattered per unit time, and as the scattered waves contain no net momentum, the scattered waves remove an amount of quasimomentum

$$-(b/c)\langle\sigma_{zy}v_x\rangle_{av}, \quad (21)$$

per unit time from the impinging wave.

Now, according to Eq. (19), the total decrease of quasimomentum in the crystal due to the dislocation-elastic wave interaction is

$$\rho b \langle \dot{u} v_x \rangle_{av} \text{ per unit time.} \quad (22)$$

For the plane wave we have the relation

$$\dot{u} = -(c/\mu)\sigma_{zy}, \quad (23)$$

where  $\mu$  is the shear modulus, and inserting Eq. (23) into the expression 22 we obtain the expression 21. Thus no quasimomentum  $G_y$  is given up to the screw, and it experiences no radiation force.

It must be emphasized that the above results do not alter our previous conclusions about dislocation mobility in an isotropic flux of thermal waves,<sup>3</sup> even though the Nabarro model involving a Lorentz force was employed. In practical cases the screw is constrained to move on one slip plane. A Lorentz force would then be of no consequence as it would be balanced out by the constraint, and a complete electromagnetic analogy can then be used. The previous calculations should be looked upon as illustrations of what happens in practical cases. When the incident wave strikes the dislocation normally to the direction of uniform dislocation motion, the retarding force felt by the dislocation is the same as that previously deduced.

Finally it should be mentioned that it is not straightforward to extend the foregoing analysis to edge dislocations. The coordinates  $x$  and  $y$  are "embedded" coordinates, i.e., they refer to a coordinate network that deforms with the crystal. In the case we have considered this leads to no complication, since the  $z$  coordinate does not enter and all displacements are in the  $z$  direction. With edge dislocations this simplicity would not exist.

**DEMONSTRATION THAT A TRUE LORENTZ-FORCE ON SCREWS INVOLVES AN EXTERNAL CONSTRAINT ON THE SCREW CORE**

Only because of the term  $\frac{1}{2}\rho\dot{u}^2$  in Eq. (12) is quasimomentum not generally conserved during screw dislocation movement. It is an interesting possibility then, that if by external constraint we keep  $\dot{u}=0$  at the dislocation core, a true Lorentz force on the screw will arise.

The wave equation of the medium is

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2}, \quad c = \left(\frac{\mu}{\rho}\right)^{\frac{1}{2}}. \quad (24)$$

If we make the Lorentz transform

$$\begin{aligned} x' &= \beta(x - v_x t), \\ y' &= y, \\ t' &= \beta(t - v_x x/c^2), \end{aligned} \quad (25)$$

where

$$\beta = (1 - v_x^2/c^2)^{-\frac{1}{2}}.$$

Equation (24) does not change form, and in cylinder coordinates  $r'$  a solution is

$$u = A \{J_0(kr') - iI_0(kr')\} e^{i\omega t'}, \quad k = \omega/c. \quad (27)$$

$J_0$  and  $I_0$  are Bessel functions of the first and second kind, respectively, and the solution represents outgoing waves far out.

When  $kr' \ll 1$ , and requiring that  $u = u_0$  when  $r' = r_0'$ , we obtain asymptotically for the real part

$$u = \frac{u_0}{\ln kr_0'} \ln kr' \sin \omega t'. \quad (28)$$

In the subsequent analysis it should be understood that we only retain terms which dominate as  $r_0' \rightarrow 0$ .

Transforming back to  $x, y, t$ , we obtain the solution

$$u = \frac{u_0}{\ln kr_0'} \ln kr' \sin[\beta\omega(t - v_x x/c^2)]. \quad (29)$$

The derivative of the logarithm does not contribute to the *average* velocity around  $r' = r_0'$ . With the conditions such that the point  $r' = 0$  is at  $x = 0$  when  $t = 0$ , the average velocity for  $r' = r_0'$  is

$$\dot{u}_0 = \beta u_0 \omega \cos(\omega t/\beta). \quad (30)$$

Expanding  $u$  in  $\xi$ , where

$$x = v_x t + \xi, \quad (31)$$

Eq. (28) becomes

$$u = \frac{u_0}{\ln kr_0'} \ln kr' \sin(\omega t/\beta) - \frac{\beta u_0 v_x \xi}{c^2} \frac{\ln kr'}{\ln kr_0'} \cos(\omega t/\beta). \quad (32)$$

The first term in Eq. (32) is symmetric around the singularity and gives rise to no uniform shear stress over the surface  $r' = r_0'$ . However, the second term will give rise to such a uniform shear stress because of the linearity in  $\xi$ . The logarithm can be regarded as a constant. So, over the surface  $r' = r_0'$  we obtain a uniform shear stress,

$$\sigma_{zx} = \mu(\partial u/\partial \xi)_{r'=r_0'} = -(\mu \beta u_0 v_x / c^2) \cos(\omega t/\beta), \quad (33)$$

or, by Eq. (30),

$$\sigma_{zx} = -\mu v_x \dot{u}_0 / c^2. \quad (34)$$

Now, choosing  $\dot{u}_0 = -\dot{u}$ , where  $\dot{u}$  now means the average velocity which the core matter would have if no external constraint on the core was present, we obtain

$$\sigma_{zx} = \mu v_x \dot{u} / c^2 = \rho v_x \dot{u}. \quad (35)$$

A positive screw at the singularity (Burgers vector  $+b$  referred to the  $+z$  direction) would then experience a force per unit length

$$F_y = -\sigma_{zx} b = -\rho b v_x \dot{u}, \quad (36)$$

which is just what is given by Eq. (3).

### CONCLUSION

Because (1) only shear stress forces can move screw dislocations; and because (2) total quasimomentum is not generally conserved when a screw able to move in all directions interacts with an elastic sound disturbance; we must conclude that the term, "a Lorentz force on screws," should be excluded from dislocation theory. Otherwise confusion will result. Only if an external constraint is applied to the matter along the screw dislocation core to keep the displacement velocity zero, does a true Lorentz-type force appear.

### ACKNOWLEDGMENTS

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