Shock wave theory for rupture of rubber

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This article presents a theory for the rupture of rubber. Unlike conventional cracks, ruptures in rubber travel faster than the speed of sound, and consist in two oblique shocks that meet at a point. Physical features of rubber needed for this phenomenon include Kelvin dissipation and an increase of toughness as rubber retracts. There are three levels of theoretical description: an approximate continuum theory, an exact analytical solution of a slightly simplified discrete problem, and numerical solution of realistic and fully nonlinear equations of motion.

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Introduction— Rapidly moving cracks in brittle materials under tension have a number of common characteristics. They cannot move faster than the shear wave speed \[ c_s \], and often exhibit a limiting velocity around half that value because of instabilities of the crack tip \[ 1,2 \]. Stresses near the tip rise in a universal singularity as \[ 1/\sqrt{r} \]. In this Letter, I show that ruptures in rubber are different. They are supersonic. There is stress enhancement but no stress singularity near their tips. They constitute a new sort of failure mode that combines characteristics of shocks and cracks.

The motivation for this study comes from experiments showing that cracks in rubber travel faster than the shear wave speed \[ c_s \]. Planar shock fronts in rubber were previously observed by Kolsky \[ 3 \]. It has not been clear how to interpret the experiments because the large nonlinearities of rubber invalidate immediate comparison with the customary theory of linear elastic fracture mechanics. In particular, one assumption of conventional fracture mechanics is that material ahead of a crack tip is strained by a vanishingly small amount, while in popping rubber the strains are several hundred percent.

Intersonic tensile cracks have been observed in numerics of Buehler, Abraham and Gao \[ 4 \]. In their calculations, this behavior is produced by a rise in sound speed near the crack tip. Here the mechanism is different; there is no rise in sound speed. Instead, two other physical ingredients work together both in numerical simulations and in analytical calculations to reproduce the basic experimental observations. First and most important, the equation of motion for rubber includes dissipation of the Kelvin form; Langer \[ 5 \] has observed that such terms may permit supersonic motion. Second, the rubber must be able to sustain larger stresses when it is relaxed along one axis than when it is stretched equally in all directions.

Continuum Theory of Rubber— Strains in rubber are several hundred percent at rupture and one must use nonlinear elastic theory to describe the situation. Sound speeds in rubber are adequately described \[ 1,2 \] by one of the most familiar free energies for non-linear elastic solids, the one due to Mooney and Rivlin \[ 6,7,8,9,10 \]. For this free energy, define the Lagrangean strain tensor \[ \epsilon_{\alpha\beta} \] :

\[
\epsilon_{\alpha\beta} \equiv \frac{1}{2} \left[ \sum_{\gamma} \frac{\partial u_\gamma}{\partial r_\alpha} \frac{\partial u_\gamma}{\partial r_\beta} - \delta_{\alpha\beta} \right].
\]

Here \( \bar{u}(\bar{r}) \) describes the distance from the origin of a mass point that was located at \( \bar{r} \) before the rubber was stretched up. From this strain tensor one can define three rotationally invariant quantities, which are \( I_1^{3D} = \text{Tr} E, \ I_2^{3D} = \sum_{\alpha<\beta} [E_{\alpha\alpha}E_{\beta\beta} - E_{\alpha\beta}^2], \) and \( I_3^{3D} = \det E \). The Mooney–Rivlin theory says that the free energy density of rubber is

\[
U/\rho \equiv w = a(I_1^{3D} + bI_2^{3D}),
\]

where \( U \) has units of energy per volume, \( \rho \) is mass density, \( a \) is a constant with units of velocity squared, and \( b \) is dimensionless. For a thin sheet of rubber, one can replace the three–dimensional theory by an effective two–dimensional one, using the facts that rubber is highly incompressible \[ 9 \], and that one can neglect all the components of the strain tensor \( E_{\alpha\beta} \) except for \( E_{zz} \). In two dimensions one has only two invariants,

\[
I_1 = E_{xx} + E_{yy}, \quad I_2 = E_{xx}E_{yy} - E_{xy}^2,
\]

and using incompressibility to solve for \( E_{zz} \) one finds

\[
E_{zz} = \frac{1}{4} \left( \frac{1}{I_2 + 2I_1 + 1} - 1 \right).
\]

Thus one obtains an effective two–dimensional Mooney–Rivlin theory

\[
w(I_1, I_2) = a(I_1 + bI_2 + E_{zz}(1 + bI_2)).
\]

For large strains, \( E_{zz} \) becomes negligibly small compared to \( E_{xx} \) or \( E_{yy} \). However, as rubber relaxes to equilibrium, the terms proportional to \( E_{zz} \) become important. They are what ensure that \( \bar{u} = \bar{r} \) is a minimum energy state.

For studying the rupture of rubber, the energy density in Eq. \( 5 \) is both too simple and too complicated. It is too simple because it does not account for the fact that when rubber is stretched enough, the polymers pull apart and the force between adjacent regions drops irreversibly to zero. It is too complicated because the terms involving \( I_2 \) and \( E_{zz} \) produce nonlinear equations of motion that are impossible to solve analytically. Therefore, to analyze the problem, I will pursue two different routes. First, I will discuss numerical routines that supplement Eq. \( 5 \) with information about rupture, toughening, and dissipation, and produce supersonic solutions. Second, I will isolate from Eq. \( 5 \) terms that are sufficient to produce good agreement with numerics and experiment, while simplifying matters enough to permit analytical solution.
Numerical System—To study rubber rupture numerically, consider a collection of mass points $u_i$ whose equilibrium locations lie on a triangular lattice, and that are connected with bonds to nearest neighbors. Take the lattice spacing of the unstretched configuration to be $\Delta$. For numerical representation of the strain invariants, let $\vec{u}_{ij} = \vec{u}_j - \vec{u}_i$, let $n(i)$ refer to the nearest neighbors of $i$, and define

$$ F_i = \frac{1}{6} \sum_{j \in n(i)} \left( \frac{\vec{u}_{ij} \cdot \vec{u}_{ij} - \Delta^2}{\lambda_f^2 - \Delta^2} \right) \quad \text{if } u_{ij} < \lambda_f $$

$$ G_i = \frac{1}{9} \sum_{j \in n(i)} \left( \frac{(\vec{u}_{ij} \cdot \vec{u}_{ij} - \Delta^2)^2}{\lambda_f^2 - \Delta^2} \right) \quad \text{if } u_{ij} < \lambda_f $$

$$ H_i = \frac{1}{27} \sum_{j \neq k \in n(i)} h(u_{ij}) h(u_{ik}) \left( \vec{u}_{ij} \cdot \vec{u}_{ik} + 2\Delta^2 \right)^2, $$

and

$$ h(u) = 1/(1 + e^{(u-u_c)/u_e}). $$

From these numerical quantities, one can form representations of the strain invariants as follows:

$$ I_1^i = F_i / \Delta^2 $$

$$ I_2^i = (9/8) (G_i - H_i + 4) / \Delta^2, $$

and finally construct the energy from

$$ U = \sum_i mw(I_1^i, I_2^i), $$

where $m$ is the mass in a unit cell, and the energy density $w$ is given by Eq. [8]. The quantities in [6a] are chosen according to two ideas. First, they are designed so that when all bonds at a node are shorter than a critical failure extension $\lambda_f$, in the continuum approximation Eqs. [7] reproduce the strain invariants in Eq. [5]. Second, they are designed so that when bonds are stretched to an extension greater than $\lambda_f$, they break. For the three–body term in Eq. (6c), it is necessary to introduce a soft cutoff through the function $h$ described in Eq. (6d), in which $u_e$ is a parameter on the order of 0.1 that sets the scale over which contributions to the three–body term drop to zero.

Figure 1 shows an image of a steady state obtained by solving dynamical equations that follow from Eq. (8). The precise equation of motion includes dissipation of the Kelvin form, and is

$$ m \ddot{u}_i^0 = -\partial U / \partial u_i^0 + \sum_{j \in n(i)} \frac{a \beta}{3} \ddot{u}_{ij}^0 \theta(\lambda_f - u_{ij}). $$

One final rule is employed. Whenever some bond $u_{ij}$ drops to a length less than $1.5\Delta$, the failure extension $\lambda_f$ for the remaining bonds attached to nodes $i$ and $j$ increases. Without some rule of this type, the back faces of the crack disintegrate. Essentially, the back faces of the rupture act like a string under tension pulling bonds at the tip apart, and they must be able to sustain tensions sufficient to do so; for details, see Eq. (11).

Numerical solutions of Eq. (9) agree acceptably with experiment. I have tried to determine which terms in it are really needed. Progressively stripping elements from (9) I found what is most likely the simplest set of equations supporting supersonic solutions. These explain the nature of the solutions, and the conditions under which they arise.

Neo–Hookean Continuum Theory—Experimentally, the dimensionless parameter $b$ in Eq. (5) is .106, so in a first theoretical account one can set $b = 0$. For strains large enough also to neglect $E_{zz}$, Eq. (5) reduces (up to an additive constant) to the Neo–Hookean energy density

$$ w = aI_1 = \frac{\rho c^2}{2} \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial u}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial y} \right)^2 \right]^2 $$

The equation of motion that follows from this energy is (for $\alpha = x$ or $y$)

$$ \ddot{u}_\alpha = c^2 \nabla^2 u_\alpha. $$

Despite the fact that the equation of motion Eq. (11) is an ordinary wave equation, it describes large extensions. The most undesirable feature of this theory is that its ground state consists in material that has collapsed down to a point; this results from dropping the terms proportional to $E_{zz}$ from Eq. (5). However, as shown in Figure 2, rupture speeds are essentially
unaffected by the presence of these terms. The theory has the great advantage that it can be solved exactly. For crack–like solutions, with Lagrangean variables \((x, y) = \vec{r}\) one has for \(y = 0\) and \(x < 0\) the boundary condition \(\partial u_y/\partial y = 0\). Neither this boundary condition nor the equations of motion couple \(u_x\) and \(u_y\), therefore, the equations support solutions where \(u_x = \lambda_x x\) does not change in time, and the motion of the mass points is purely vertical. These solutions are identical to the solutions for a crack in anti-plane shear[13], as recorded for example in Ref. [1], p. 356. The static solution has a parabolic tip. Steady states moving at velocity \(v\), are identical to the static solution, but are Lorenz contracted in the direction of motion by a factor of \(\sqrt{1-v^2/c^2}\). As the crack speed \(v\) approaches the wave speed \(c\), the tip becomes increasingly blunt.

The wave speed \(c\) has been thought the upper speed limit for crack–like solutions of Eq. (11). However, supersonic solutions are possible if one adds Kelvin dissipation corresponding to the rightmost term in Eq. (9) to obtain for a steady state moving at velocity \(v\),

\[
v^2 \frac{\partial^2 u}{\partial x^2} = c^2 \nabla^2 u - v c^2 \frac{\partial u}{\partial x}.
\]

The variable \(u\) in this equation is the vertical motion of mass points \(u_y\); the horizontal locations of all mass points remain fixed at \(u_x = \lambda_x x\), so there is no need to keep track of them further. Supplemet Eq. (12) with the boundary conditions

\[
\frac{\partial u}{\partial y} = \frac{\partial^2 u}{\partial x \partial y} \quad \text{for} \quad x < 0; \quad u = 0 \quad \text{for} \quad x > 0.
\]

\[
u \rightarrow \lambda_y y \quad \text{as} \quad y \rightarrow \infty .
\]

Solutions of Eq. (12) can be obtained with the Wiener–Hopf technique[14]. One has the following results for the upper face of the rupture where \(y = 0^+\) and \(x < 0\):

\[
\frac{\partial u}{\partial x} \bigg|_{x=0} = -\int_0^0 dx' \frac{\lambda_y e^{x/v\beta}}{\sqrt{-\pi v/3x(v^2/c^2 - 1)}}.
\]

and

\[
\frac{\partial u}{\partial y} \bigg|_{y=0} = \frac{\lambda_y e^{x/v\beta} v/c}{\sqrt{v^2/c^2 - 1}}.
\]

Therefore, the slope \(\alpha\) of the back face of the rupture seen in the lab is

\[
\frac{-\lambda_y}{\lambda_x \sqrt{v^2/c^2 - 1}}.
\]

This is the slope of a shock cone trailing an object traveling at speed \(v > c\) in a medium of wave speed \(c\). Note that the velocities \(v\) and \(c\) are measured in a Lagrangean reference frame described by variables \(x\) and \(y\). Horizontal and vertical speeds measured in the laboratory are larger by factors of \(\lambda_x\) and \(\lambda_y\) respectively; this geometrical fact accounts for the factor \(\lambda_y/\lambda_x\) in (15a). The vertical strain at the origin is obtained by setting \(x = 0\) in Eq. (13). One obtains a simple but approximate prediction for rupture speed by checking when only one of two crack-line bonds has snapped, and horizontal forces on crack-line atoms do not balance to zero, while in the analytical solutions, all forces in the horizontal direction are ignored.

\[
\lambda_x \quad \text{and} \quad \lambda_y
\]

\[
\text{respectively; this geometrical fact accounts for the factor } \lambda_y/\lambda_x \text{ in (15b). The vertical strain at the origin is obtained by setting } x = 0 \text{ in Eq. (13). One obtains a simple but approximate prediction for rupture speed by checking when bonds angled at } 60^\circ \text{ in a triangular lattice reach their breaking point } \lambda_f :\]

\[
\lambda_f^2 = \frac{1}{4} \lambda_x^2 + \frac{3}{4} \left[ \frac{\partial u}{\partial x} \bigg|_{(0,0)} \right]^2
\]

\[
\Rightarrow \lambda_y = \sqrt{\frac{4(\lambda_f^2 - \lambda_x^2)}/3}.
\]

In order to compare with experiment, there is a single free parameter to fix, which is the breaking point \(\lambda_f\). Figure 2 shows a comparison of the predictions from Eqs. (13) with experimental and numerical data, using \(\lambda_f = 5.5\).

| \(\lambda_f/\sqrt{(4\lambda_f^2 - \lambda_x^2)/3}\) |
|---|
| Experiment |
| Discrete Solution, \(N = 2000\) |
| Direct integration, \(N = 200\) |
| Continuum Approximation |

An additional interesting quantity to check is the distance squared between horizontal mass points behind the rupture. It is

\[
\lambda_x^2 + \frac{\lambda_y^2}{v^2/c^2 - 1} = \frac{4}{3} \lambda_f^2 + \frac{2}{3} \lambda_x^2 - \lambda_y^2.
\]
This quantity exceeds $\lambda_f^2$ for characteristic values of $\lambda_f$, $\lambda_x$, and $\lambda_y$, which explains why it is necessary for $\lambda_f$ to increase behind the rupture if the back surface is not to disintegrate.

**Neo–Hookean Discrete Theory**—Not only can the continuum Neo–Hookean theory be solved, but the discrete theory, Eq. 9 can also be solved exactly, provided in Eq. 5 one sets $b = 0$ and $E_{zz} = 0$. The solution involves the application of methods described in Refs. 15, 16, 17, and details will be presented elsewhere. Figure 2 shows exact solutions for rupture speeds in systems 200 and 2000 rows high compared both with direct integration of the equations of motion and experiment. In addition to removing discrepancies between the very simple results in Eqs. 15 and numerics, solving the discrete model explains the conditions under which one gets supersonic or subsonic solutions for cracks in tension.

The basic result is this: including dissipation through $\beta$ in the equation of motion introduces a length scale $\beta c$ into the problem. The behavior of cracks hinges on the ratio of $\beta c$ to the lattice spacing $\Delta$. When $\beta c/\Delta$ is much less than one, cracks behave as in conventional fracture mechanics, and their speed is limited from above by $c$, except within a very narrow window of strains where all bonds in the system ahead of the crack approach their breaking point. As $\beta c/\Delta$ approaches and exceeds one, dissipation progressively destroys the stress singularity around conventional crack solutions, but at the same time it permits the appearance of supersonic solutions. Note in Eq. 15 that rupture speed is determined by vertical extension $\lambda_y$, rather than by the total energy stored ahead of the crack tip as in conventional fracture mechanics. Exact solution of the discrete Neo–Hookean theory shows that 15 is not completely accurate, but its scaling properties are correct. One sees in Figure 2 that the relation between rupture velocity and system extension $\lambda_y$ has essentially reached the macroscopic limit for systems 200 rows high and velocities $v$ above 1.05c. The macroscopic limit is subtle near $v = c$, since solutions with speeds above and below $c$ scale differently as system size goes to infinity.

Establishing the existence of supersonic ruptures in tension opens up many possibilities for future work. The supersonic ruptures in experiment begin to oscillate once $\lambda_x$ exceeds a critical value. The numerical and analytical tools provided here should provide an appropriate starting point for studying the oscillations. Finally, it would be interesting to know if there are materials different from rubber that meet the conditions needed to sustain supersonic ruptures.

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