NEW SCENARIO FOR FRICTION

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ABSTRACT

We show that fixed-length cracks can race along an interface between two dissimilar crystals pressed together in compression and shear. These cracks permit one crystal to slide over the other as expected from Coulomb's laws of friction. We calculate the coefficient of static friction to be 0.2.

KEYWORDS

Fracture, friction, Coulomb's law, interfaces

INTRODUCTION

Many problems familiar to continuum mechanics can be studied in a new way when one decides to take into account explicitly the atomic structure of matter. Reluctance to take this path largely stems from the assumption that inclusion of atomic detail will create an impenetrable barrier to analytical progress. This assumption is best reversed by counter–examples. We show here that it is possible to calculate a coefficient of friction analytically starting with an atomic description of sliding surfaces.

Coulomb's laws of friction say that the force needed to slide a solid across a surface is proportional to the force with which the two are pushed together, but independent of the apparent area of contact. This fact is surprising. One would expect that solids in contact over larger areas would become more difficult to slide. Conventional explanations are based upon the fact that actual areas of contact are much smaller than apparent. The contacts are made through populations of asperities that jut out of the two solids, and the actual area of contact grows in proportion to the force pressing them together[1].

The complexities of this conventional explanation make it difficult to study in great detail. The asperities are treated in statistical fashion, and their individual properties are usually described phenomenologically. We therefore think it will be of interest to display a case where frictional sliding can be described analytically, and with a level of detail reaching down to the atomic scale.

We are able to accomplish this task because our scenario of frictional sliding is different from the conventional one. Our picture of solids in contact does not include asperities. Instead, we imagine two perfect crystals pressed into one another, weakly adhered across an interface, and ask what horizontal force is necessary for the first to begin to slide over the second. The answer is that sliding begins when the ratio of shear to compressive force reaches a critical value. At this point it becomes possible for fixed-length cracks to form at the interface, and propagate at a substantial fraction of the speed of sound, allowing one surface to slip over the other. Cracks of this sort were first described by Yoffe[2], for whom they were a mathematical artifact making it possible to describe dynamic cracks. The condition for these interface cracks to form is completely independent of the

area of contact of the two crystals. Therefore this scenario, like the conventional one, leads to a slipping rule in accord with Coulomb's law of friction.

The objection will naturally be raised that this scenario, even if correct, is irrelevant. Real surfaces are rough, the conventional picture applies, and ours is just a theoretical curiosity. To counter this objection, we appeal to experiment. Propagating modes similar in character to those appearing in our theories have been observed in laboratory studies of sliding[3, 4]. The idea that such modes exist plays an important role in geophysics, where traveling pulses of slip are invoked to explain anomalously low generation of heat during earthquakes[5, 6, 7, 8, 9, 10, 11, 12]. Thus while we agree that our calculations take place in an idealized setting, we believe that sliding of this sort can actually occur. We do not know how large is the domain of validity for our picture of sliding dominated by self-healing Yoffe cracks, as opposed to sliding dominated by the flow and failure of asperities.

CALCULATIONS

Establishing our idealized picture of friction involves combining information from several different calculations.

Our first calculation describes the motion of a semi-infinite crack along a weak interface between a crystal and a rigid substrate. This work is performed analytically for arbitrarily large systems, using Wiener-Hopf techniques as in Slepyan[13] and Marder[14]. The techniques must be generalized because certain symmetries present in the earlier problems are now lost. The Wiener-Hopf problem for interface cracks becomes a 2×2 system of coupled equations that can be solved using Wilson's algorithm[15]. The end result is an analytical description of the motion of every atom, and in particular a relationship between the speed of the semi-infinite interface crack and loading conditions far away.

Semi-infinite cracks traveling along interfaces exhibit the peculiar phenomenon of stress rotation, first found by Williams [16], and schematically shown in Figure 1 where the bottom material is assumed rigid for simplicity.

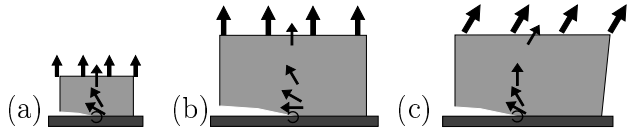

Figure 1: Stresses rotate near the tip of a crack separating dissimilar materials. Samples (b) and (c) are each twice the size of sample (a). The top boundaries in (a) and (b) have similar displacements while the the near-tip stress fields in (a) and (c) are similar.

Suppose one pulls straight up on a sample containing a crack as in Figure 1(a). Linear elastic theory predicts a counter-clockwise rotation of stress fields from the boundary to the crack tip. The rotation is logarithmically slow, progressing a constant amount as the distance to the tip is halved. The rotation halts just outside the tip, where the continuum approximation fails. Now consider a similar thought experiment on a sample twice as high [Figure 1(b)] but with the same inter-atomic separation. Because the continuum approximation is valid over a larger portion of the sample, there is more room for stress rotation, and as a result, the near-tip stress fields in Figure 1(b) are just a rotated version of those in Figure 1(a).

Because of the existence of stress rotation it is possible to construct cracks whose tip experiences tension even though far away the system is loaded in compression. In all such cases, the crack opens for some distance behind the tip, but the compressive loading then forces the upper and lower crack surfaces back into contact. Thus, these cracks are propagating regions of slip and separation of a sort first envisioned by Yoffe[2].

Our second calculation is an explicit computation of such cracks, using molecular dynamics simulations, as shown in Figure 2. Unfortunately, the systems that are accessible numerically are small, involving only millions of atoms. Increasing to billions of atoms is possible, but would not help much, since stress rotation is logarithmically slow.

Our third calculation is an analytical calculation for moving cracks of finite length on interfaces. We rederived and generalized the continuum solution of Dhaliwal, Saxena, Das, and Patra [17, 18] for a Yoffe crack

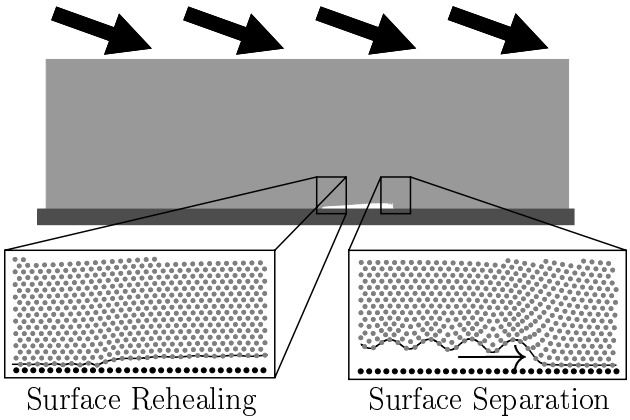

Figure 2: Numerical simulation of a self-healing Yoffe crack traveling through a compressed strip.

moving along an interface. In the continuum solution one chooses crack velocity v, crack length l, the total distance with which the surfaces slip Δu, and the far field stresses $(\sigma_{xy}^{\infty}, \sigma_{yy}^{\infty})$. These parameters determine a unique solution.

The history of self-healing Yoffe interface cracks has been controversial[19, 20, 21, 22, 23], because the continuum descriptions of these cracks contain disturbing features, including infinite numbers of self-intersection of opposing crack faces, and energy fluxes to crack tips in unphysical directions. We propose to resolve these controversies by locating those continuum cracks that are consistent with our atomic-scale solutions near the tips.

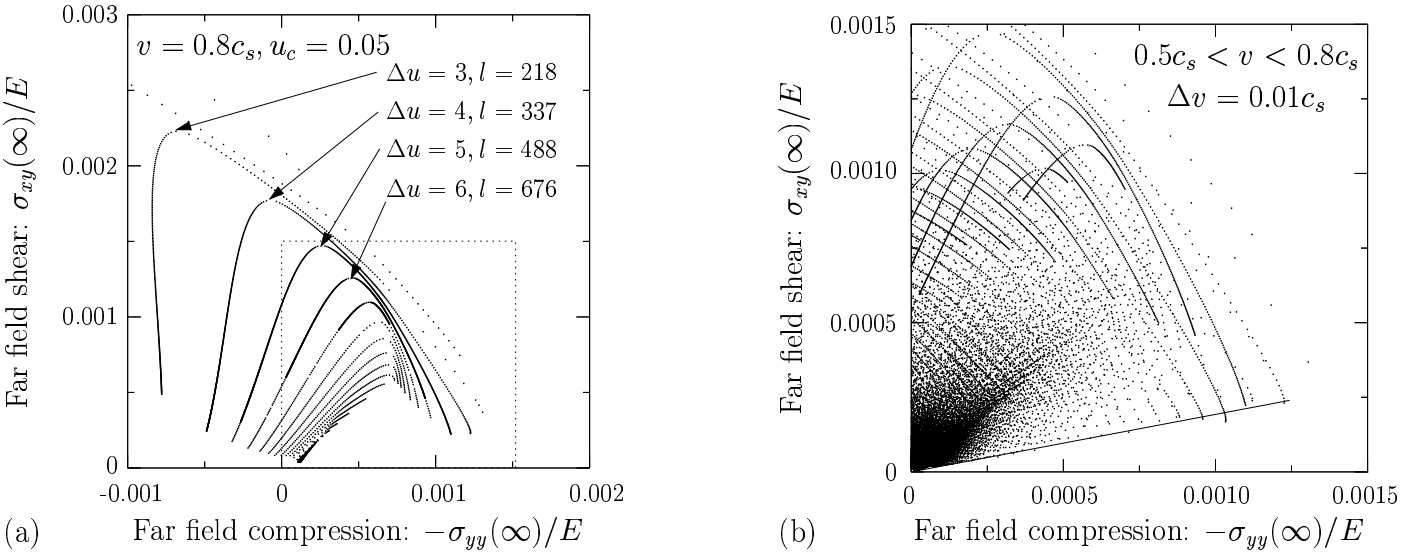

Figure 3: Shear and tensile stresses that support steadily moving Yoffe cracks. Stresses are normalized by Young's modulus E and velocities are normalized by shear wave speed c_s. Integral values of crack length l and total slip Δu lead to a discrete set of states for each velocity. (a) Solution set for $v = 0.8c_s$. Points that appear to form a curve have the same slip Δu but different crack lengths l. (b) Catalog of 120,000 interface crack states, for velocities between 50% and 80% of the shear sound speed, in increments of 1%. Notice that when the ratio of stresses $-\sigma_{xy}/\sigma_{yy}$ drops below around 0.2 there are no more states.

Thus our final calculation connects microscopic and macroscopic scales. We compute the far-field asymptotic stresses of the semi-infinite atomic interface cracks and demand that these stresses match the near-field asymptotic stresses for the continuum self-healing Yoffe cracks. Only a small fraction of the original continuum solutions turn out to be consistent with microscopic constraints on near-tip physics. We find that the original five-dimensional space of continuum solutions is reduced to a space indexed by one continuous parameter (the velocity) and one countably infinite parameter (crack length and slip).

The set of solutions shown in Figure 3(a) results from setting crack velocity $v = 0.8c_s$ (where c_s is the shear

wave speed) and exhaustively considering all possible crack lengths l and slips Δu. In Figure 3(b) we display all running crack states for velocities below 80% c_s, in increments of 1% c_s. When the ratio of horizontal shear to compressive shear $-\sigma_{xy}/\sigma_{yy}$ drops below around 0.2 there are no more states. Thus the condition for sliding to become possible corresponds to Coulomb's law of friction, with a coefficient of 0.2.

QUESTIONS

Many questions have still to be addressed. When does this mechanism of friction apply, and when does flow and fracture of asperities dominate? How do the conditions for initiation of these Yoffe cracks differ from conditions of propagation? Could such a difference account for a difference between coefficients of static and kinetic friction? How can effects of temperature and surface roughness be incorporated within this scenario?

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