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Designer shocks for carving out microscale surface morphologies

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Shockwaves are propagating disturbances with a long history of study in gas dynamics, fluid dynamics and astrophysics. We also see examples of shocks in everyday life such as a traffic jam in which the oncoming traffic has much lower density than the cars within the traffic jam. A classical compression wave involves propagation of a discontinuity in which information is absorbed from both sides in the shock layer. Undercompressive shocks are more unusual - they have special properties including the transfer of information through the shock and often different stability properties than their compressive cousins. In the past decade, undercompressive waves have been studied in micro and nanoscale applications in which surface forces dominate the physics in the shock layer. These forces can permit the existence of undercompressive waves and their utility is just now coming to fruition. Perkinson et al [1] demonstrate how to utilize undercompressive shocks in ion-bombarded surfaces to create patterns with steep ridges on the micron scale.

The traffic jam example is one that can be modeled with a simple one dimensional first order nonlinear wave equation, or `conservation law' introduced in the mid 1950s [2,3]:

$$u_t + f(u)_x = 0. \tag{1}$$

Here u is the material being transported in the direction x and f is the flux of the material. A shock is a solution to such an equation with a discontinuity in u that travels with speed s given by the Rankine-Hugoniot jump condition

$$s = \frac{f(u_L) - f(u_R)}{u_L - u_R}.$$

Such models can be solved exactly for any choice of states u_L and u_R on the left and right of the discontinuity. All such shockwaves are compressive - meaning that they satisfy an entropy condition; the speed s of the shock is faster than the characteristics speed $f'(u_R)$ ahead of it and slower than the speed $f'(u_L)$ behind it. It was traditionally thought that any physical process described by such a simple one-dimensional model could have only compressive shocks. This fact can be proved rigorously in the case where the physics in the shock layer is ``diffusion'' or Brownian motion, as is seen in gas dynamics. The modification of equation (1) to include linear diffusion in the shock layer is

$$u_t + f(u)_x = u_{xx} \tag{2}$$

With diffusion, shock discontinuities are smoothed, however the basic shock structure, including the speed of the shock as determined by eq. (1), are exhibited in smooth traveling wave solutions of (2). More recently a number of `scalar law' physical systems have been identified that produce under-compressive shocks. The model considered by Perkinson et al [1] involves an equation of motion for the slope of the surface of the form (1) with additional physics in the shock layer from surface diffusion, resulting in a model similar to (2) with additional fourth order diffusion on the right hand side. A one dimensional nonlinear model for ion-beam

sputtering was introduced in 2005 by Chen et al [4] who showed that it produced undercompressive shocks that could be reproduced in experiments. The model is a conservation law in which u is the slope of the surface and the nonlinear flux function *f* is the yield function, which gives the average velocity of erosion of the surface as a function of its local slope, and is, in general, non-convex. Their model has a fourth order term that models additional smoothing effects such as Mullins-Herring surface diffusion or ion-enhanced viscous flow confined to a thin surface layer. They showed that stable steep undercompressive waves were experimentally viable in ion bombarded surfaces with common physical parameters.
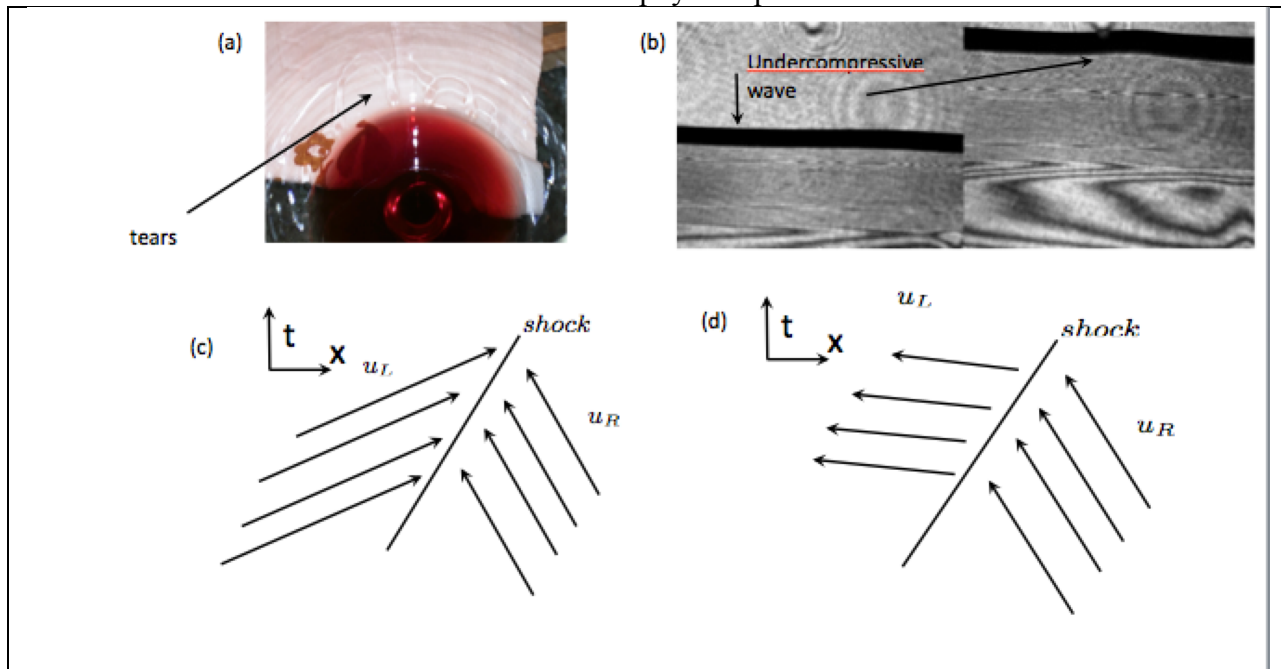

Fig 1. (a) tears of wine ;(b) an undercompressive- compressive shock pair in a thermally driven coating flow showing two successive snapshots in time. The undercompressive shock is thick and dark indicating a steep change in height using interferometry [11] ; (c) characteristic diagram of a compressive shock; (d) characteristic diagram of an undercompressive shock.

In the case of compressive shocks, information travels into the shock from both sides. This is illustrated in figure 1 c. In the case of an undercompressive shock, information enters the shock from one direction only (fig 1d). It will generally pass through the shock and exit the shock on the other side. Undercompressive shocks can arise in one-dimensional conservation laws when the correct physics in the shock layer is something other than second-order diffusion. Mathematical examples were first constructed for diffusive-dispersive equations but without any direct comparison to physical experiments [5]. About 10 years ago a set of experiments involving driven thin films confirmed the presence of undercompressive shocks in micron-scale coating flows driven by thermal gradients [6]. For such systems, the dominant physics in the shock layer was not diffusion but rather surface tension on the air liquid interface of the free surface of the film. Compressive shocks in driven films are well-known; the most common example is the case of paint dripping down a wall under the flower of gravity. Such systems are known to have instabilities, namely the classic fingering instability that causes the paint to drip rather than flowing as a uniform front [7]. This is the same mechanism that leads to the formation of tears of wine (fig 1a), in which the driving mechanism is a Marangoni stress caused

by a gradient in surface tension which is due to a gradient in the alcohol concentration in the meniscus on the wineglass because of differential evaporation of the alcohol [8,9,10].

In order to have an undercompressive shock in a one-dimensional scalar conservation law one needs two ingredients: (a) a nonconvex flux f for the bulk flow and (b) some kind of higher order physics in the shock layer such as surface tension. The non-convex flux typically results from two competing physical effects in the driving mechanism - for example a surface stress and a bulk force in opposite directions. In the case of ion bombarded surfaces, the nonconvexity is in the yield function. For both fluid films and ion bombarded surfaces, the physics in the shock layer comes from surface tension or surface energies resulting in a mathematical model with fourth order diffusion. For such systems, undercompressive shocks are not generic. For weak shocks, in which the values u_L and u_R are close together, one expects a compressive shock even with fourth order rather than second order diffusion. The tears of wine example and the paint dripping example both correspond to this case. Undercompressive shocks can occur when the jump reaches a threshold and crosses a change in convexity of the flux. Moreover, undercompressive shocks do not exist for a finite range of parameters u_L and u_R; the theory predicts that for a given right state u_R there is an isolated value of u_L for the undercompressive wave. This means that such shockwaves are often accompanied by a companion wave in the form of a compressive shock or rarefaction fan in order to transition to the background material. It also means that any driving mechanism for undercompressive waves will trigger a specific wave with a known prescribed jump across the shock.

Another feature of compressive waves in driven films is that they tend to be unstable to transverse perturbations. The capillary ridge caused by surface tension is unstable to a beading effect leading to paint dripping or instabilities in spin coating at high rotation speeds. These drips need to be controlled in any kind of design manufacturing process. One exciting aspect of the initial discovery of undercompressive shocks in thin films was their stability to transverse perturbations thus creating a new stability mechanism for a driven coating process. However, that idea has not led, to date, to a stable design procedure for liquid coating processes. There are other examples of undercompressive shocks in coating flows including a very commonly observed phenomenon of water being pushed up the windshield of the car by the surface stress of the wind counterbalanced by gravity. Such behavior is potentially relevant to important applications like deicing of airplane wings [12].

In Holmes-Cerfon et al [13] it was proposed that two undercompressive waves could be collided to form isolated steep ridges. A fully two dimensional experiment was realized in a magnesium alloy under uniform irradiation by a focused ion beam. The results compared well to fully two-dimensional simulations of the nonlinear model [14]. In Perkinson et al [1] the authors show that this design principal can be used to solve an inverse problem – given a prescribed desired end-state with connected ridges, they successfully used the undercompressive waves to carve out the desired pattern. In order to solve the inverse problem, a one dimensional nonlinear model, in the form of a diffusive Hamilton-Jacobi equation, was developed for the nonlinear motion of the undercompressive ridge as it evolves. Monte Carlo simulations were carried out to identify the best choice of initial pit to create the final state using ion-bombardment. The low-dimensional evolution model for the transverse motion of the shock was an instrumental in solving this inverse problem because it allows for a lower dimensional set space of initial configurations for

testing.   This new work shows that such unusual wave patterns can be used to control design features in small scale materials applications.   Moreover the authors present new mathematical analysis that leads to a simplified one-dimensional model that accurately describes the fully two-dimensional motion of the front, a crucial feature needed to utilize undercompressive waves for design.   This works has ramifications for both technological design procedures and new simplified model development for two-dimensional effects in nonlinear wave propagation.

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