Shock-Front Broadening in Polycrystalline Materials

John L. Barber, Kai Kadau, T-14

Consider a polycrystalline solid comprising numerous grains, where each grain is composed of a different crystallographic orientation of some material. If a shock is induced at one side of the material and subsequently penetrates into the polycrystal, how does the initially sharp shock front grow in width with time? Meyers [1,2] has proposed a model in which the major contribution to the shock-front broadening comes from the differences in shock speed that distinct points on the shock front experience as they move through different grains. This model explicitly ignores other effects, such as scattering at grain boundaries, which may also influence the evolution of the shock-front width. The aim of this work is to explore the mathematical implications of the Meyers model, and to derive a useable analytical expression for the shock-front width.

Figure 1 shows a schematic representation of our polycrystal, along with an illustration of the coordinate system to be used. The shock front is assumed to originate on one face of the polycrystal, at $y = 0$, and penetrate into the bulk of the solid. Different points on the shock front propagate independently in straight lines in the $+y$ direction, their speeds at any given location determined by the properties of the grain they are passing through. A particular sample ray arrives at a location $y = x$ after a propagation time t. Since the geometry of the grains and the shock speeds therein are generally random, the relationship between x and t will be a random one. If the shock-front speed as a function of position for a sample ray is $v(y)$, then the propagation time to reach x is

$$t = \int_0^x dy \frac{1}{v(y)} = \frac{x}{c} + \int_0^x dy \left(\frac{1}{v(y)} - \frac{1}{c} \right), \quad (1)$$

where

$$c = \left\langle \frac{1}{v} \right\rangle^{-1} \quad (2)$$

is the reciprocal of the average inverse shock speed of the material, averaged over both the random grain geometry and the distribution of shock speeds within each grain. This is the overall rate at which the shock front will move through the crystal.

According to (Eq. 1), the propagation time can be separated into the sum of a deterministic part and a random part with mean zero. Using a version of the central limit theorem, it can be shown that in the limit of large x, the integral in (Eq. 1) reduces to a Gaussian random variable (RV), such that

$$t = \frac{x}{c} + \left(2x \int_0^\infty dy \chi(y) \right)^{\frac{1}{2}} Z \quad . \quad (3)$$

Here $\chi(y)$ is the spatial autocorrelation function of the integrand in (Eq. 1) and Z is a standard normal deviate.

Equation (3) gives the propagation time as a RV in terms of a fixed penetration distance x. By solving (Eq. 3) for x, we may obtain the random penetration distance as a function of fixed time t. The resulting relation can be manipulated to yield a relationship between the shock-front position x (i.e., the average value of x) and the shock-front width (i.e., twice the standard deviation of x):

$$\frac{\Delta x}{d} = \left(\frac{8c^2}{d} \int_0^\infty dy \, \chi(y) \right)^{\frac{1}{2}} \left(\frac{\bar{x}}{d} \right)^{\frac{1}{2}} . \quad (4)$$

Here we have introduced d, a measure of the average grain diameter, in order to render (Eq. 4) scale invariant.

As it stands, (Eq. 4) is completely general, though unwieldy, since it requires complete knowledge of the autocorrelation function $\chi(y)$. We can obtain a more useable relation by making the additional assumption that the shock speed within each grain is

uncorrelated with the geometry of the grains themselves. In this case, it can be shown that (Eq. 4) reduces to

$$\frac{\Delta x}{d} = \left[4c^2\chi(0)\frac{d^*}{d}\left(1+\frac{\sigma^2}{d^{*2}}\right)\right]^{\frac{1}{2}}\left(\frac{\bar{x}}{d}\right)^{\frac{1}{2}}, \quad (5)$$

where d^* and σ are known in stochastic geometry as the average chord length and standard deviation of the chord length, respectively [3]. Note that for the common special case of a Poisson Voronoi lattice in three dimensions, where d is taken as the mean caliper length [4], we have

$$\frac{d^*}{d}\left(1+\frac{\sigma^2}{d^{*2}}\right) = 0.631. \quad (6)$$

The expression (Eq. 5), along with a choice for the distribution of shock speeds within the polycrystal, yields a testable prediction for the dependence of the shock-front width on shock position. By simulating the model directly, we can test the steps leading up to (Eq. 5). The results of several such simulations for various system widths L are shown in Fig. 2. The shock speed distribution and grain geometry were chosen to be consistent with a sample of polycrystalline iron at equilibrium in a body-centered cubic state, with a 3-D Poisson Voronoi geometry. We see that to within noise the simulation results are consistent with the theoretical prediction (Eq. 5). More realistic polycrystalline simulations using the embedded atom method [5,6] are currently being performed, in order to verify how well the assumptions and predictions of this model compare with a real physical system.

For more information contact John L. Barber at jlbarber@lanl.gov.

[1] M.A. Meyers and M.S. Carvalho, *Mater. Sci. Eng.* **24**, 131 (1976).
[2] M.A. Meyers, *Mater. Sci. Eng.* **30**, 99 (1977).
[3] D. Stoyan, et al., *Stochastic Geometry and its Applications* (Wiley, 1995).
[4] A. Okabe, et al., *Spatial Tesselations: Concepts and Applications of Voronoi Diagrams* (Wiley, 1992).
[5] K. Kadau, et al., *Science* **296**, 1681 (2002).
[6] K. Kadau, et al., *Phys. Rev. B* **72**, 064120 (2005).

Funding Acknowledgments
Laboratory Directed Research and Development Program.

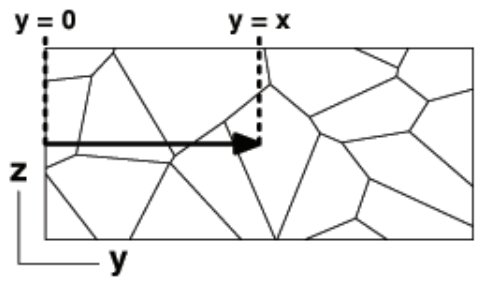

Fig. 1.
A schematic representation of the coordinate system in our polycrystal. The arrow indicates the direction of shock propagation.

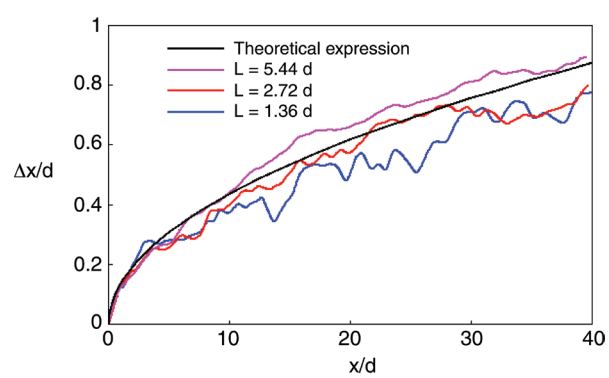

Fig. 2.
Results for the evolution of the shock-front width, as determined by direct simulation of the ray model. Shown are curves for various values of the system width L.