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Dynamic scaling in a simple one-dimensional model of dislocation activity

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ABSTRACT

We examine a simple one-dimensional (1D) model of dislocation activity, including a stress-activated source and mutually interacting dislocations. We demonstrate, through numerical and analytical steps, that the dislocations emitted from a 1D stress-activated source evolve towards a distribution which is self-similar in time, and we derive the power-law forms and distribution function. We show that the asymptotic distribution is a step function, and the dislocation front moves out linearly in time. The spacing between dislocations in the asymptotic distribution is uniform and increases logarithmically in time. The number of dislocations increases as $t/\ln(t)$, and the strain increases as $t^2/\ln(t)$.

§ 1. INTRODUCTION

Similiarity solutions in dislocation problems have been studied for decades. Dislocation pile-ups, for example, were some of the first such problems to be addressed with similarity solutions (Head 1972a, b, c). Recent work used scaling theory to explore the Hall–Petch relation for a dislocation source in multilayers (Friedman and Chrzan 1998) and cell patterning (Shim *et al*. 2001, Hahner 2002). Scaling relationships can often be established for the effects of governing parameters such as time, finite size, external stress and source activation stress. Such general forms, an example being the Hall–Petch relation (Hirth and Lothe 1982), are of particular importance for understanding of the general behaviour of dislocations under a variety of conditions.

The dynamic similarity condition (or scaling form) (Barenblatt 1996) assumes that the dislocation distribution is self-similar in time, so that the distribution at one time is related to itself at other times by $n(x, t) = \phi(t)\, g(x/\psi(t))$. A simple example of a dynamic similarity solution is given in the case of the free expansion of a set of

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interacting straight parallel dislocations, all of the same Burgers vector and on the same slip plane. In this case, the dislocation density $n(x, t)$ evolves according to

$$\frac{\partial n(x,t)}{\partial t} + \frac{\partial n(x,t)v(x,t)}{\partial x} = 0 \tag{1}$$

and the (overdamped) velocity comes from the self-interactions of the dislocations:

$$v(x,t) = \int_{-\infty}^{\infty} \frac{\mathcal{P}}{x-y} n(y,t)\,\mathrm{d}y. \tag{2}$$

Head (1972a, b, c) showed that the similarity solution for this problem is of the form

$$n(x,t) = \frac{1}{t^{1/2}}\, g\left(\frac{x}{t^{1/2}}\right), \tag{3}$$

with

$$g(p) = \begin{cases} \dfrac{1}{2\pi}(4N - p^2)^{1/2}, & p^2 < 4N, \\ 0, & p^2 > 4N, \end{cases} \tag{4}$$

where N is the number of dislocations.

The similarity solution (for the free expansion problem and in general) is more than a special solution involving particular initial conditions. Rather, it corresponds to the asymptotic behaviour of the general solution (Barenblatt 1996). That is, for a given initial condition $n(x, 0) = n_0(x)$, the solution $n(x, t)$ at long times evolves asymptotically to the similarity solution.

While some recent work has focused on the behaviour of sources in finite-sized regions, this paper considers a simpler problem: a single stress-activated source in an infinite medium. We demonstrate numerically and analytically that this model exhibits scaling solutions and interpret the general dynamics of the dislocations in terms of the scaling form. Given the amount of work in this area, it is somewhat surprising that this problem does not appear to have been addressed previously in publications. However, the simplicity of the problem allows the scaling solutions to be obtained with relative ease and for the general utility of the scaling solution to be demonstrated. Because of its general importance, it is useful to publish the solution for this simple case.

§2. Simple one-dimensional problem

We use a familiar (Weertman 1957, Rosenfield and Hahn 1968, Yokobori *et al.* 1974) simple model of dislocation activity which addresses a stress-activated source of overdamped interacting dislocations.

An external stress σ is exerted on a source (at $x = 0$), which emits individual dislocations (figure 1). The dislocations are emitted in pairs; the dislocations at $x > 0$ have Burgers vector magnitude b, and at $x < 0$ have the opposite† Burgers vector magnitude $-b$.

† Of course, for such a single source, the opposing dislocations have opposite line directions and the same Burgers vector magnitudes. The same forces are created by considering that all dislocations in this model have the same line directions and opposite Burgers vector magnitudes.

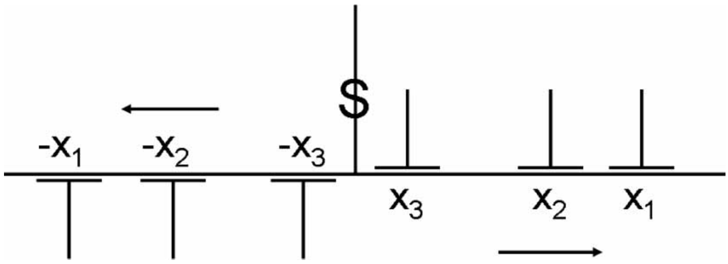

Figure 1. A simple 1D model of dislocation activity. A stress-activated source emits dislocations in pairs which expand away from the source along a line.

Once created, the dislocations move according to dissipative law

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \gamma b_i \left(\sigma + \mu \sum_{j \neq i} b_j f(x_i - x_j) \right), \tag{5}$$

where μ is the elastic modulus, and the force on each dislocation is the sum of the external force σb_i and interactions with the other dislocations. The damping factor for the dislocation motion is γ.

The force between dislocations in a linear elastic continuum varies as the inverse distance. Of course, when the dislocations are close together, as they are at the source, the continuum force is incorrect. To simplify the numerical calculations, we chose a general form for the (mutual) force of dislocations separated by a distance z,

$$f(z) = \frac{z}{z^2 + a^2}, \tag{6}$$

which introduces a (lattice) constant a, characteristic of the distance at which the continuum result breaks down. The introduction of this (small) length scale a is equivalent to performing the principal value in the integral in equation (2) by

$$\frac{\mathcal{P}}{z} \rightarrow \frac{z}{z^2 + a^2}$$

and then taking the limit after the integration as $a \rightarrow 0$.

The source creates a new pair of dislocations at $x = 0$. (No numerical problems result because the interaction force (6) is well behaved at short distances.) The mutual attraction of this pair reaches a maximum of $1/2a$ at $x = a/2$. The older dislocations (i.e. those emitted earlier and that are farther from the source) exert a repulsive force on the newer dislocations (a 'back stress'), which tends to inhibit the separation of the newest pair. If the external force can overcome the forces tending to keep the pair together, then the pair separates. When the region near the source is cleared, a new pair is created at the origin and the process continues.

Given these equations of motion, the measure of slip is

$$\Lambda = 2 \sum_i x_i,$$

where the sum is only over one half of the dislocations (those for $x_i > 0$). (The strain would be Λ divided by some characteristic length of the sample, such as the size of the sample or the distance between sources.) The elastic energy stored in the dislocation array is (again, the same convention on the sums)

$$U = \frac{\mu b^2}{2} \sum_{ij} \log\left(\frac{(x_i + x_j)^2 + a^2}{(x_i - x_j)^2 + a^2}\right).$$

It is useful to consider the continuum form for the same system, which is written in terms of the dislocation density $n(x, t)$:

$$\frac{\partial n}{\partial t} + \frac{\partial (nv)}{\partial x} = R(t)\delta(x), \tag{7}$$

with

$$v(x, t) = \lim_{a \to 0}\left[b\,\mathrm{sgn}(x)\left(\sigma + b\int_{-\infty}^{\infty} \frac{x - y}{(x - y)^2 + a^2} n(y, t)\,\mathrm{sgn}(y)\,\mathrm{d}y\right)\right] \tag{8}$$

and $R(t)$ is the rate of emission of dislocations from the source. In the continuum form the number is $N = 2\int_0^{\infty} n(x, t)\,\mathrm{d}x$, the measure of slip is $\Lambda = 2\int_0^{\infty} xn(x, t)\,\mathrm{d}x$, and the strain energy is

$$U = \lim_{a \to 0}\left[\frac{\mu b^2}{2}\int_0^{\infty}\int_0^{\infty} n(x, t)n(y, t)\log\left(\frac{a^2 + (x + y)^2}{a^2 + (x - y)^2}\right)\mathrm{d}x\,\mathrm{d}y\right].$$

A power-law scaling form

$$n(x, t) = t^{\alpha} g\left(\frac{x}{t^{\beta}}\right) \tag{9}$$

would imply that

$$\begin{aligned} N(t) &\propto t^{\alpha+\beta}, \\ \Lambda(t) &\propto t^{\alpha+2\beta}, \\ U(t) &\propto t^{2\alpha+2\beta}, \end{aligned} \tag{10}$$

which are straightforward to check numerically.

The discrete equations were integrated numerically with a straightforward approach. The simulated time is limited by the $O(N^2)$ nature of the problem and so was limited to N of the order of 10^5. Good energy conservation was used as the criterion to determine the optimal time step.

The exponents α and β were then obtained by comparing the numerical results with the time dependences of N, Λ and U (equations (10)). Using a linear fit of the log–log plots (figure 2), we determined that $\beta = 1.0$ and $\alpha \approx -0.10$. We found, however, that, while the value of β does not depend on the length of the simulation, the value of α does. The longer the simulated time, the closer α approaches zero from below. We shall show analytically in the next section that t^{α} in the scaling form should properly be $1/\ln(t)$.

The numerical dislocation distributions (figure 3) were then scaled according to equation (9). As is seen in the figure, the scaled distributions almost overlap. This data collapse and the fact that two exponents give a good fit to the three functions above are supportive of the idea that the system has evolved to a self-similar state.

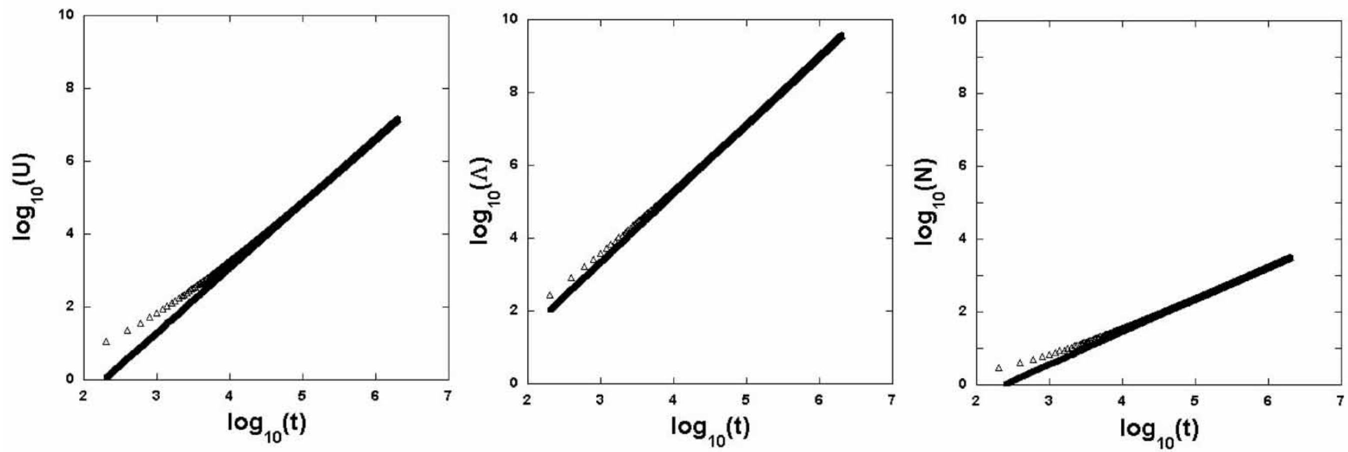

Figure 2. The numerical data and the linear fits of the log–log plots for Λ, N and U versus t. The numerical solutions asymptotically approach a power-law form (i.e. straight lines on this plot).

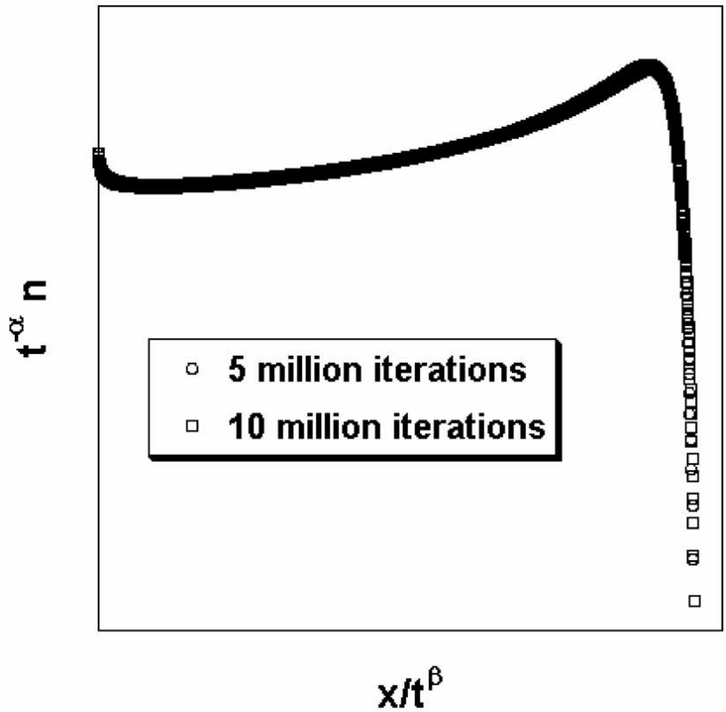

Figure 3. Numerical dislocation distributions at two different times. The distributions are scaled to illustrate the data collapse.

§ 3. Scaling analysis

Some simple arguments will give us the particular values of the scaling exponents α and β. Note first that the spacing between dislocations goes like n^{-1}; in particular, for fixed values of x/t^{β} the spacing $\lambda \propto t^{-\alpha}$. Because the mutual repulsions cause the dislocation array to expand, we have $\alpha \leqslant 0$.

Given that α is non-positive, it is simple to show that $\beta = 1$ in the problem at hand as long as the external stress is on. Consider $\dot{\Lambda} = 2\int_0^{\infty} x[\partial n(x,t)/\partial t]\,\mathrm{d}x$, which from the equation of evolution is

$$\dot{\Lambda} = \sigma b N(t) + 2\mu b^2 \int_0^{\infty}\int_0^{\infty} n(x,t)\left(\frac{x-y}{(x-y)^2+a^2} - \frac{1}{x+y}\right) n(y,t)\,\mathrm{d}x\,\mathrm{d}y. \tag{11}$$

According to the scalings (10), the left-hand side scales as $t^{\alpha+2\beta-1}$. The terms on the right-hand side scale as $t^{\alpha+\beta}$ and $t^{2\alpha+\beta}$, respectively. The dominant term on the right-hand side is that due to the external stress, and this shows $\beta = 1$.

The value for α and the function g are interdependent. Consider the situation where the source is turned off; then number conservation (equations (10)) requires that $\alpha = -\beta$. With the source turned on, we must consider the details of how the source operates, which is determined by the distribution of dislocations. The rate of dislocation emission is $R \propto \dot{N} \propto t^{\alpha}$. Because the back stress produced by existing dislocations tends to slow the creation of new dislocations, it should be that α has a negative value, perhaps approaching zero from below, which would be like a logarithmic dependence.

To demonstrate more definitively that the proper scaling form is $n(x,t) = g(x/t)/\ln(t)$, we recall that the numerical simulations showed a distribution function which resembles a step function. Such a distribution function is equivalent to assuming that the spacing between dislocations is uniform (although dependent on time). This is reasonable, because the mutual repulsions tend to distribute the distributions evenly. We shall show that the assumption of equal spacing leads to $R \propto 1/\ln(t)$, and that this rate in turn produces a step-function distribution.

Let us examine the function of the source under the assumption that all existing dislocations are spaced evenly by a distance $\lambda(t)$. Consider the net force on a member of the newest pair. The external force can overcome the mutual attraction of the pair, but this is undone by the back stress produced by the other older dislocations. The next-youngest dislocation created by the source must move sufficiently far away for that back stress to diminish enough for the newest pair to be pulled apart. That next-youngest dislocation must move a distance λ before the newest pair will be allowed to move out. At precisely that moment, the net force on the newest pair at $x = d = a/2$ is zero; so

$$\sigma b - \frac{\mu b^2}{2d} = -\mu b^2 \sum_{m=1}^{N} \left(\frac{1}{d - m\lambda} - \frac{1}{d + m\lambda} \right)$$
$$\propto \mu b^2 \left[\frac{2}{\lambda}[C + \ln(N)] + \frac{2d^2}{\lambda^3}\zeta(3) + \mathrm{O}\left(\frac{d}{\lambda}\right)^4 \right], \tag{12}$$

where C is Euler's constant. Retaining the dominant term for large t (or, equivalently, N), we can solve for λ to obtain

$$\lambda(t) = \frac{\tilde{\sigma}}{2\mu b \ln[N(t)]}, \tag{13}$$

where $\tilde{\sigma} = \sigma - \mu b/2d$ is the value of the threshold stress above threshold. The rate of creation is proportional to λ^{-1}; so

$$\frac{\mathrm{d}N}{\mathrm{d}t} \propto \ln[N(t)] \tag{14}$$

or

$$N(t) \propto \frac{t}{\ln(t)}. \tag{15}$$

Comparison with the scaling forms (10) shows clearly that the t^{α} should be replaced by $1/\ln(t)$.

Taking now $n(x,t) = g(x/t)/\ln(t)$ and substituting into the evolution equation gives

$$(f - p)g'(p) + \frac{-g(p) + [h(p)g(p)]'}{\ln(t)} = \delta(p), \tag{16}$$

where $p = x/t$, $f = \sigma b$ and

$$h(p) = \lim_{a \to 0} \left[\int_0^{\infty} g(q) \left(\frac{p - q}{(p - q)^2 + a^2} - \frac{1}{p + q} \right) \mathrm{d}q \right]. \tag{17}$$

For large t, the $1/\ln(t)$ term drops out, and the distribution must satisfy $(f - p)g'(p) = 0$, which gives a step function. Hence we have a consistent solution.

There is one subtlety, however, which concerns the behaviour of $g(p)$ as p approaches f. In this case the coefficient of the $1/\ln(t)$ term in equation (16) is divergent because of the singular derivative of $g(p)$ at $p=f$. The problem ultimately arises in the transition from the discrete to continuum descriptions and does not present any real physical difficulty here. The simplest way to demonstrate that the solution is acceptable is to look at moments of the distribution function, which we do in the next section. By using integrated quantities, rather than derivatives, the transition to continuum description is smooth and there are no special problems at the end of the distribution.

Thus, the scaling solution for this problem is

$$n(x,t)=\frac{c(\sigma)\theta(\sigma bt/\gamma-x)}{\ln(t)}. \tag{18}$$

The logarithmic scaling is consistent with the numerical results which showed that the effective time exponent tended to zero from below, and that the convergence was very slow. The analysis is instrumental in showing the asymptotic behaviour of the numerical solutions.

§4. Crossover and asymptotic solutions

It is also instructive to consider the cross-over behaviour implied in the logarithmic terms in equation (16). These correspond to the evolution of the distribution function, which asymptotically approaches the scaled distribution. The distribution obtained from the numerical simulations is not exactly a step function. The analysis here implies that the distribution should slowly (i.e. logarithmically) approach the scaled distribution (a step function).

The evolution of the distribution from some initial or special conditions to the scaled distribution as an asymptotic form is expected to hold generally for all problems of this type. This can be seen from the evolution equation for $n(x,t)$ or, equivalently (and more easily), it can be demonstrated from the evolution of the spatial moments of n.

Consider first the simpler case of free expansion of an array of positive straight parallel dislocations. In this case, the evolution equation is as equation (7) with $R=0$ but with only the mutual interactions; so

$$v(x,t)=\int_{-\infty}^{\infty}\frac{\mathcal{P}}{x-y}n(y,t)\,\mathrm{d}y. \tag{19}$$

Multiplying the evolution equation by x^m and integrating gives the evolution of the mth moment in terms of lower moments. The even moments follow

$$\dot{\mu}_m(t)=\frac{m}{2}\sum_{r=0}^{m-2}\mu_r(t)\mu_{m-2-r}(t), \tag{20}$$

which is solved in terms of their initial values by

$$
\begin{aligned}
&\mu_0(t) = N, \\
&\mu_2(t) = \mu_2(0) + N^2 t, \\
&\mu_4(t) = \mu_4(0) + 4Nt\mu_2(0) + 2N^3t^2, \\
&\mu_6(t) = \mu_6(0) + 6Nt\mu_4(0) + 3t\mu_2(0)^2 + 15N^2t^2\mu_2(0) + 5N^4t^3, \\
&\quad etc.
\end{aligned}
\tag{21}
$$

From this it is clear that the initial values of the moments do not influence the asymptotic values, which are $\mu_{2p} \propto N^{p+1}(4t)^p\Gamma(p+1/2)/(\pi^{1/2}\Gamma(p+2))$. These are precisely the moments of the scaled distribution (equation (3)), showing that the general solution asymptotically approaches the self-similar state. It is also clear from equation (21) that the moments approach their asymptotic values as $1/t$.

Although the details are more involved, the same general statement holds for the source problem. In that case, the even moments satisfy

$$\dot{\mu}_m(t) = fm\mu_{m-1}(t) + m\sum_{r=0}^{m-2}\mu_r\mu_{m-2-r}, \tag{22}$$

while the odd moments are somewhat more involved:

$$\dot{\mu}_m(t) = fm\mu_{m-1}(t) + \tfrac{1}{2}\left(m\sum_{r=0}^{m-2}\mu_r\mu_{m-2-r} + K_m\right), \tag{23}$$

with

$$K_m = m\int_0^\infty\int_0^\infty n(x)n(y)\frac{x^{m-1}+y^{m-1}}{x+y}\,\mathrm{d}x\,\mathrm{d}y. \tag{24}$$

Using the scaling form shows that $K_m = C_m(ft)^m/[\ln(t)]^2$ with $C_m < 2$ for all m. The dominant term in these equations is that produced by the external force. Keeping only those terms, the moments become

$$\mu_m(t) \propto \frac{(ft)^{m+1}}{(m+1)\ln(t)}, \tag{25}$$

which are precisely those derived from the similarity solution (equation (18)). This demonstrates clearly that the distribution function evolves asymptotically into the similarity solution. One can also observe that the moments approach their asymptotic values as $1/\ln(t)$, as expected from the numerical results.

§ 5. Conclusions

We have demonstrated, through numerical and analytical steps, that the dislocations emitted from a 1D stress-activated source evolve towards a distribution which is self-similar in time. The asymptotic distribution is a step function, and the front moves out linearly in time. The spacing between dislocations in the asymptotic distribution is uniform and increases logarithmically in time. The number of dislocations increases as $t/\ln(t)$, and the strain increases as $t^2/\ln(t)$.

We believe that this behaviour is characteristic of dislocation-source problems in general and expect that our approach should be useful in more complex systems.

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