Slip line growth as a critical phenomenon

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We study the growth of slip line in a plastically deforming crystal by numerical simulation of a double-ended pile-up model with a dislocation source at one end, and an absorbing wall at the other end. In presence of defects, the pile-up undergoes a second order non-equilibrium phase transition as a function of stress, which can be characterized by finite size scaling. We obtain a complete set of critical exponents and scaling functions that describe the spatiotemporal dynamics of the slip line. Our findings allow to reinterpret earlier experiments on slip line kinematography as evidence of a dynamic critical phenomenon.

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dislocations is given by
\[
\chi \frac{dx_i}{dt} = b_i + \sum_{j=1 \atop j \neq i}^{N} \sigma_{i,j}^\text{int} + \sigma_{i}^\text{img} + \sum_{P} f(x_i - X_P),
\]
where \(\chi\) is an effective viscosity and \(\sigma\) is the external stress. The interaction stress \(\sigma_{i,j}^\text{int}\) between dislocations \(i\) and \(j\) is computed taking into account the image stresses of dislocation \(j\) due to the open boundary conditions, while \(\sigma_{i}^\text{img}\) is due to the interaction between dislocation \(i\) and its own images. A compact expression of the interaction and image stresses can be obtained by performing the sum over the images \((22)\), yielding
\[
\sigma_{i,j}^\text{int} = -\frac{\pi \mu b_j}{2L} \left[ \cot \left( \frac{x_j - x_i}{2L} \right) + \cot \left( \frac{x_j + x_i}{2L} \right) \right],
\]
\[
\sigma_{i}^\text{img} = \frac{\pi \mu b_i}{2L} \cot \left( \frac{x_i}{L} \right),
\]
where \(\mu\) is the shear modulus, \(k = \pi\) for screw dislocations and \(k = 2\pi(1 - \nu)\) for edge dislocations, \(\nu\) is the Poisson ratio. We notice here, that the sum over the images is exact only in the case of screw dislocations. For edge dislocations, there is an additional subdominant correction scaling as \(1/r^2\) that we neglect here since it should not influence the scaling behavior. The last term in Eq. (1) represents the interactions with pinning centers placed at randomly chosen positions \(X_P\) with \(P = 1, ..., N_P\). The detailed shape \(f(x)\) of the individual pinning force is inessential for most purposes, provided it is of short-range nature, and in this case it is given by
\[
f(x) = -f_0 \frac{x}{\xi_P} e^{-\left(x/\xi_P\right)^2},
\]
where \(\xi_P\) is the range of the interaction and \(f_0\) controls its strength.

Dislocations are typically generated by Frank-Read like sources, which can only be represented in a three dimensional model. In lower dimensions, it is customary to model the source phenomenologically by creating dislocations with a certain rate. The drawback of this approach is that the new dislocation produces an artificial discontinuity in the stress field. To overcome this problem, we employ a method suggested by Zaiser [21] in which a source is represented by an immobile dislocation, placed at position \(x_1\), with a time-dependent Burgers vector \(b_1(t)\) growing with stress. When \(b_1(t) = b\), a new mobile dislocation is emitted from the source whose Burgers vector is reset to zero. The evolution equation for \(b_1(t)\) is given by
\[
\chi_1 \frac{db_1}{dt} = \theta(\sigma_1^\text{eff}) \sigma_1^\text{eff},
\]
where \(\theta\) is the Heaviside step function and \(\chi_1\) is a damping constant that we set equal to \(\chi_1 = \chi/b\). The effective stress \(\sigma_1^\text{eff} = \sigma + \sigma_1^\text{int} + \sigma_1^\text{img}\) is the sum of the constant external stress \(\sigma\), the stress \(\sigma_1^\text{int}\) produced by the interaction between the source and the mobile dislocations (including the relative images), and the stress \(\sigma_1^\text{img}\) produced by the interaction between the source and its own images. These stresses are obtained from Eq. (2) observing that \(\sigma_1^\text{int} = \sum_{j=2}^{N} \sigma_{i,j=1}^\text{int} + \sigma_1^\text{img} = \sigma_1^\text{img}\).

Integrating numerically Eqs. (1) and (4) we analyze the dynamics of the pile-up as a function on the external stress \(\sigma\) and the system size \(L\). The units of time, space, and forces are chosen so that \(b = 1, \chi = 1\) and \(\mu/k = 1\). For the simulations reported here, we considered parameters \(L = 256, 512, 1024, 2048, 4096, 8192, x_1 = 16\) and the pinning centers are Poisson distributed with an average spacing \(d_p = L/N_p = 2\) with \(f_0 = 1\) and \(\xi = 1\). From the experimental point of view, a key quantity describing the growth of the slip line is the plastic strain rate \(\dot{\varepsilon}\) given by
\[
\dot{\varepsilon} \equiv \frac{1}{L} \sum_i b_i \dot{x}_i = b \rho v,
\]
where \(\rho = N/L\) is the dislocation density and \(v = \sum \dot{x}_i/N\) is the average dislocation velocity. Notice that all these quantities are defined per unit dislocation length, given the effective one dimensional geometry of our model.

Since the strain rate is simply the product of the dislocation density and average velocity, we study directly these two quantities. We find that after an initial transient the density and the velocity reach a steady state.
value ($\rho_s$ and $v_s$ respectively) that depends on the system size $L$ and the applied stress $\sigma$ as shown in the inset of Fig. 2. The graphs are suggestive of a non-equilibrium phase transition controlled by the stress between a pinned phase at low stress and a moving phase at large stresses. The curves become sharper close to the depinning point as $L$ is increased, as expected when finite-size effects are present. To confirm this idea we perform a scaling collapse according to

$$
\rho_s(\sigma, L) = L^{-\alpha/\nu} f[(\sigma - \sigma_c)L^{1/\nu}],
$$

(6)

$$
v_s(\sigma, L) = L^{-\beta/\nu} g[(\sigma - \sigma_c)L^{1/\nu}],
$$

where the scaling function $f(u)$ fulfills the limits

$$
f(u) \simeq \begin{cases} 
1 & \text{if } u \ll 1, \\
u^\alpha & \text{if } u \gg 1,
\end{cases}
$$

(7)

and for $g(u)$ they are

$$
g(u) \simeq \begin{cases} 
1 & \text{if } u \ll 1, \\
u^\beta & \text{if } u \gg 1.
\end{cases}
$$

(8)

The best collapse is obtained using $\sigma_c = 1.05 \pm 0.05$, $\nu = 2.85 \pm 0.05$, $\alpha/\nu = 0.35 \pm 0.02$ and $\beta/\nu = 0.17 \pm 0.02$, as shown in Fig. 2. These exponent combinations correspond to $\alpha = 1.00 \pm 0.02$, $\beta = 0.48 \pm 0.02$, and yield a scaling form for the strain rate of the type

$$
\dot{\varepsilon}(\sigma, L) = L^{-(\alpha+\beta)/\nu} h[(\sigma - \sigma_c)L^{1/\nu}],
$$

(9)

where $h(u) = f(u)g(u)$, as we have also verified directly.

We have also analyzed the slip line growth dynamics in the transient regime. The time dependence of the dislocation density and velocity can also be characterized by finite size scaling functions which at the critical point $\sigma = \sigma_c$ are given by

$$
\rho(t, L) = L^{-\alpha/\nu} f_t[t/L^{z}],
$$

$$
v(t, L) = L^{-\beta/\nu} g_t[t/L^{z}],
$$

(10)

where $z$ the dynamic exponent. The best collapse is obtained for $z = 1.25 \pm 0.02$ as shown in Fig. 3. The scaling functions, for small values of the argument, scale as $f_t(u) \sim u^\zeta$, with $\zeta = 0.55 \pm 0.05$ and $g_t(u) \sim u^{-\theta}$, with $\theta = 0.10 \pm 0.05$. Hence, the strain rate in the initial phase grows as $\dot{\varepsilon}(t) \sim t^{\zeta - \theta}$. Notice that the scaling exponents are considerably different from what is expected for a regularly spaced pileup with periodic boundary conditions, where the density is constant (hence $\alpha = 0$) and the critical exponents are $\beta \simeq 0.78$, $z \simeq 0.78$ and $\nu \simeq 1.5$.

To elucidate the role of the boundary condition and characterize the internal morphology of the pile-up, we report in Fig. 4 the stationary density $\rho_s(x, L)$ and velocity $v_s(x, L)$ profiles for different values of the system size $L$. The data collapse is consistent with the scaling hypothesis in Eq. 6 with the exponents $\beta = 0.48 \pm 0.02$ and $\nu = 2.85 \pm 0.05$. The best collapse is obtained using $\sigma_c = 1.05$. The best collapse is obtained for $\alpha/\nu = 0.35 \pm 0.02$, $\beta/\nu = 0.17 \pm 0.02$ and $z = 1.25 \pm 0.02$ which is consistent with the scaling collapse in Eq. 2.
size $L$, for $\sigma = \sigma_c = 1.05$. We observe inhomogeneities for both density and velocity profiles which can be described as power laws: $\rho_s(x, L) \sim x^{-\gamma}/L^{\psi}$ and $v_s(x, L) \sim x^{\phi}/L^\beta$, with $\gamma \approx 0.25 \pm 0.02$, $\psi \approx 0.09 \pm 0.02$ and $\phi \approx 0.42 \pm 0.02$. These behaviors are consistent with the scaling of the stationary density and velocity in the critical regime.

Hence, we have the scaling relation $\gamma + \psi = \alpha/\nu$, that is verified by the numerical values of the exponents. Similarly, from the steady-state velocity equation

$$v_s(\sigma_c, L) = \frac{1}{L} \frac{\int_0^L \rho_s(x, L) v_s(x, L) dx}{\int_0^L \rho_s(x, L) dx} \sim L^{-(\phi - \gamma)}$$

we obtain the relation $\phi - \gamma = \beta/\nu$, which is again in agreement with our numerical estimates.

In conclusion, we have studied the slip line formation at the initial stage of plastic deformation in a crystal by means of the double-ended pile-up model finding that in presence of pinning centers (quenched disorder) the model exhibit a non-equilibrium phase transition. As a consequence of this dislocation density, velocity and strain-rate are described by finite size scaling. Finite size scaling has direct implications for size effects: the size dependence of the yield stress $\sigma_Y$ observed in micron scale plasticity \cite{2}. Considering the scaling law in Eq. \ref{eq:scaling} we expect that the yield stress for finite $L$ grows towards the asymptotic value $\sigma_0$ according to $\sigma_Y(L) = \sigma_0 - A/L^{1/\nu}$, where $A$ is a positive constant. This type of inverse size effect, with the strength increasing with the sample size, is due to the larger back-stress exerted on the source by the pile-up as its length is increased. In more general cases, involving many sources and several slip lines, the constant $A$ is expected to be negative as shown in other models of the yielding transition \cite{1}.

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References

\begin{enumerate}
\item M. Zaiser, Adv. Phys. \textbf{55}, 185 (2006).
\item M. D. Uchic, D. M. Dimiduk, J. N. Florando, and W. D. Nix, Science \textbf{305}, 986 (2004).
\item D. M. Dimiduk, C. Woodward, R. LeSar, and M. D. Uchic, Science \textbf{312}, 1188 (2006).
\item F. F. Csikor, C. Motz, D. Weygand, M. Zaiser, and S. Zapperi, Science \textbf{318}, 651 (2007).
\item J. Weiss and J. R. Grasso, J. Phys. Chem. B \textbf{101}, 6113 (1997).
\item M.-C. Miguel, A. Vespignani, S. Zapperi, J. Weiss, and J. R. Grasso, Nature \textbf{410}, 667 (2001).
\item R. F. Tinder and J. P. Trzil, Acta. Metall. \textbf{21}, 975 (1973).
\item H. H. Pothoff, Phys. Stat. Sol. (a) \textbf{77}, 215 (1983).
\item H. Godon, H. H. Potoff, and H. Neuhauser, Cryst. Latt. Def. \textbf{19} 373 (1984).
\item A.J. Liu and S.R. Nagel, Nature \textbf{396}, 21 (1998).
\item M. Kardar, Phys. Rep. \textbf{301}, 85 (1998).
\item F. R. N. Nabarro, Proc. R. Soc. London, Ser. A \textbf{381}, 285 (1982).
\item S. Zapperi and M. Zaiser, Mater. Sci. Eng., A \textbf{309-310}, 348 (2001).
\item M.-C. Miguel, A. Vespignani, M. Zaiser, and S. Zapperi, Phys. Rev. Lett. \textbf{89}, 165501 (2002).
\item M. Zaiser and P. Moretti, J. Stat. Mech. \textbf{P08004} (2005).
\item H. Neuhauser, in \textit{Dislocations in Solids} Vol.6, Edited by F. R. N. Nabarro (North-Holland, Amsterdam, 1983).
\item H. Neuhauser, O. B. Arkan, and H. Flor, Czech. J. Phys. B \textbf{38}, 511 (1988).
\item O. B. Arkan and H. Neuhauser, Phys. Stat. Sol. (a) \textbf{99}, 385 (1987).
\item P. Moretti, M.-C. Miguel, M. Zaiser, and S. Zapperi, Phys. Rev. B \textbf{69}, 214103 (2004).
\item M. F. Kanninen and A. R. Rosenfield, Phil. Mag. \textbf{20}, 569 (1969).
\item M. Zaiser, private communication.
\item J. P. Hirth and J. Lothe, \textit{Theory of Dislocations} (Wiley & Sons, New York, 1984).
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