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Controlling Strain Bursts and Avalanches at the Nano-to-Micro Scale

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We demonstrate, through 3-dimensional discrete dislocation dynamics simulations, that the complex dynamical response of nano and micro crystals to external constraints can be tuned. Under load rate control, strain bursts are shown to exhibit scale-free avalanche statistics, similar to critical phenomena in many physical systems. For the other extreme of displacement rate control, strain burst response transitions to quasi-periodic oscillations, similar to stick-slip earthquakes. External load mode control is shown to enable a qualitative transition in the complex collective dynamics of dislocations from self-organized criticality to quasi-periodic oscillations.

Power-law scaling of avalanche phenomena is widely 12 observed in many nonequilibrium natural systems. 13 Examples are found in geologic earthquakes, snow 14 avalanches, sand pile slides, and strain bursts during 15 plastic flow [1, 2]. The realization that such vastly di-16 verse physical systems display common features, implies 17 scale invariance and compels a search into universal fun-18 damental laws. The common scaling raises the possibil-19 ity that the intricate system behavior can be described 20 by simple local rules, despite the complexity of the un-21 derlying internal dynamics. One concept that is widely 22 used to interpret this universality is self-organized criti-23 cality (SOC) [3]. In a SOC system, the dynamics has an 24 attractor characterized by infinite correlation time and 25 length, hence displaying scale-free scaling. A key hy-26 pothesis behind this abstraction is that the driving force 27 varying rate is much slower than the internal relaxation 28 rate [3, 4] of a system undergoing SOC. Nevertheless, 29 since this condition may not always hold, one wonders if 30 the qualitative aspects of a system's dynamical behavior 31 change when the driving force changing rate is compara-32 ble to its internal relaxation rate? Our objective here is 33 34 to investigate the relationship between the external driving force and relaxation dynamics associated with strain 35 bursts during nano- and micro-scale plastic deformation 36 of crystals. 37

At the smallest of physical scales (e.g. nano-to-38 micro scale), the release of plastic strain by intermittent 39 "bursts" has been found to belong to this power-law scal-40 ing behavior [2, 5-8]. One additionally unique aspect of 79 41 plasticity is that the driving force varying rate can be 42 experimentally tailored. Considering a simple but illus-43 trative case, a pillar is subjected to uniaxial compression 44 in Fig. 1. The force actuator, typically a voice coil, can⁸³ 45 exert an open-loop stress rate $\dot{\sigma}_0$ and/or be controlled 46 to impose a strain rate $\dot{\varepsilon}_0$. For a proportional controller 47 with stiffness K_p , the internal stress rate in the pillar is 48 [9], 49

$$\dot{\sigma} = \frac{\alpha E}{1+\alpha} (\dot{\varepsilon}_0 - \dot{\varepsilon}^p) + \frac{\dot{\sigma}_0}{1+\alpha} \tag{1}$$

where $\alpha = K_p/K$ is the relative stiffness ratio, $K = {}_{92}$ 50

EA/H is the pillar stiffness, E, A and H are the Young module, cross section area and height of the pillar, respectively. $\dot{\varepsilon}^p$ is the plastic strain rate due to all internal dislocation dynamical activities. Once the stiffness ratio α is infinitely large, or $\dot{\sigma}_0$ and $\dot{\varepsilon}_0$ are very low, $\dot{\sigma}$ becomes very sensitive to $\dot{\varepsilon}^p$, implying that the driving force changing rate ($\dot{\sigma}$) is dominated by and comparable to its internal relaxation rate $(\dot{\varepsilon}^p)$. This indicates that the corresponding slip statistics are expected to violate SOC.

However, it is generally believed that the machine stiffness K_p only contributes to the cutoff of the power law scaling [6, 8, 10]. The present investigation demonstrates that, if the machine stiffness is extremely high, dislocation avalanche dynamics (and hence strain bursts) undergo a transition from scale-free critical behavior to quasi-periodic oscillations. Interestingly, this is consistent with recent findings on the role of very slow loading rates (low $\dot{\sigma}_0$ and $\dot{\varepsilon}_0$) [11, 12], as suggested by Eq. 1. The underlying microstructure mechanism for this dynamical regime transition are disclosed. Considering that the dynamical behaviors under soft or hard machine stiffness conditions are vastly different, the corresponding intermittent plasticity will henceforth be described as either avalanche or burst, respectively. Moreover, a dislocation based branching model is proposed, giving a clear and precise physical picture of the avalanche dynamical behavior.

The vast majority of existing submicron mechanical testing experiments can only cover a narrow range of machine stiffness. In addition, the time necessary for dislocations to travel through 1 μ m sample is estimated at about 1 ns [13]. In state-of-the-art experiments, the feedback loop frequency is ≈ 78 kHz (time constant \approx 13 μ s) [8], which means that current experimental controller response rate is much slower than sample plastic relaxation rate by 4 orders of magnitude. Namely, the driving force changing rate is much slower than internal relaxation rate. Therefore, most previous experimental conditions correspond to the regime where SOC is observed. Discrete dislocation dynamics (DDD) studies, as a computer simulation tool, make it possible to supple-



FIG. 1. Simplified sketch of pillar compression. (a) Exper-137 imental setup with an open-loop (directly applying a force ¹³⁸ F_0) and closed-loop control (to realize displacement control); ¹³⁹ (b) Simulation setup, a proportional dominated closed-loop 140 control is considered here with $F_f = K_p(U_0 - U)$, which is 141 simplified as a spring with a finite machine stiffness K_p . The external stress rate $\dot{\sigma}_0 = \dot{F}_0/A$, target strain rate $\dot{\varepsilon}_0 = \dot{U}_0/H$, actual strain rate $\dot{\varepsilon} = \dot{U}/H$, where A and H are the cross section area and height of the pillar, respectively. One typical 145 dislocation configuration in a pillar with d = 3000 b is shown as an example

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ment experimental testing and explore regimes that are 149 93 currently difficult to access experimentally [6, 14]. The 150 94 current research presents the first systematic 3D-DDD 151 95 investigation on the slip statistics at submicron scale, 152 96 accounting for the effects of the interaction of an exter- 153 97 nal loading mode [15-17]. Compared with most of exist- 15498 ing two dimensional (2D) DDD studies [2, 18], the key 155 99 approximations inherent in 2D techniques are resolved. 156 100 Specifically, dislocation junction formation and destruc- 157 101 tion, and the occurrence of cross slip are all accounted 158 102 for with minimal ad hoc assumptions. 103

The simulation setup is schematically shown in Fig. 160 104 1b. We conducted simulations of compression tests on 161 105 Cu pillars of different diameters, ranging from 1000-3000 162 106 b (≈ 300 nm- 1 μ m), where b is the burgers vector mag- 163 107 nitude. The aspect ratio H/d is 3. Two extreme ma- 164 108 chine stiffness cases are first considered, corresponding 165 109 to pure strain control ($\alpha = +\infty$) and pure stress con-166 110 trol ($\alpha = 0$). Here, under pure stain control, the ap- 167 111 plied strain rate $\dot{\varepsilon}_0 = 960s^{-1}$. Correspondingly, under 168 112 pure stress control, the actual loading rate $\dot{\sigma}_0$ is $E\dot{\varepsilon}_0$. 169 113 Fifty and twenty separate simulations with different ini-170 114 tial dislocation configurations are carried out under each 171 115 loading mode for d = 1000 b and d = 3000 b, respectively. ¹⁷² 116

Figure 2a presents the results of statistical analy- 173 117 sis of the burst displacement magnitude ΔU . To ob- 174 118 tain maximum resolution of the limited simulation data 175 119 set, the complementary cumulative distribution function 176 120 (CCDF) is used. Fig. 2a clearly illustrates that ΔU , un- 177 121 der pure stress control, exhibits a well-defined power law 178 122 distribution spanning several orders of magnitude. The 179 123

power law exponent for the corresponding probability density is found to be 1.5, agreeing well with the generally accepted range of $1.35 \sim 1.67$ [5, 6, 19–21]. In addition, the power law distribution is consistent across system size, implying the existence of scale-free universality. In contrast, the CCDF of ΔU under pure strain control seems not to exhibit power-law scaling behavior for both small and large system sizes. Meanwhile, most of the data concentrate within one order of magnitude. An analogous breakdown of the power law scaling under pure strain control is also observed for the statistics of burst duration [9].

Then, how to describe the strain burst statistics under pure strain control? When discussing the temporal statistics of earthquakes, distinct dynamical behaviors are distinguished by the coefficient of variation $C = s_x/\overline{x}$ [22], where s_x and \overline{x} are the standard deviation and mean value, respectively. For the cases of C > 1 and C < 1, the distribution is referred to as "clustered" and "quasi-periodic", respectively; otherwise, if C = 1, it is a random Poisson distribution [22]. Taking the results of ΔU here, C is calculated as 1.9 and 0.9 under pure stress and pure strain control, respectively. This suggests that the dynamical behaviors under pure strain control becomes quasi-periodic. Similar to previous studies [11, 22], quasi-periodicity here is found to be stochastic, due to the intrinsic scatter induced by random cross slip or different dislocation configurations. Quasi-periodic strain bursts under pure strain control are manifested through the smoothed plastic strain rate, as clearly shown in Fig. 2b. Here, the time series of $\dot{\varepsilon}^p$ is smoothed over a fixed time window of 0.24 μ s. For comparison, the smoothed plastic strain rate under pure stress control, also shown in Fig. 2c, corresponds to a depinning phase transition.

Close examination of dislocation configuration evolution reveals that the mechanisms that control avalanche versus quasi-periodic burst behavior are significantly different, and are highly dependent on the external constraint. First, let's consider pure strain control. In the submicron regime (e.g. d = 1000 b), each strain burst is found to be dominated by sequential activation and deactivation of single arm dislocation sources. Once a source is activated, the accompanying plastic strain leads to a decrease in the stress level (see Eq. 1, $\alpha = +\infty$). Even if a weaker source is formed during one burst event, sometimes it also cannot operate due to the lower prevailing stress after relaxation. This makes it difficult to trigger simultaneous operation of multiple dislocation sources (see Fig. 3b), especially for small samples with limited volume. We have recently shown that dislocation sources themselves are transient, because they generally result from the formation of dipolar loops by cross-slip [7]. This rapid stress drop prevents the strain burst from continuously growing into a full-fledged avalanche. Consequently, large-scale cooperative interactions between



FIG. 2. (a) Statistical properties of burst displacement under 204 pure strain and stress control modes for pillar with diameters 205 d = 1000 b and 3000 b. (b-c) Typical evolution of plastic strain rate and its averaged value in 0.24 μ s windows, showing (b) quasi-periodic strain bursts under pure strain control, and (c) depinning transition dislocation avalanche under pure stress control

dislocations that can lead to SOC cannot be realized ²¹² 180 under pure strain control. Note that this discussion ap-²¹³ 181 plies to a sample size ranging from several nanometers ²¹⁴ 182 to about 1 micrometer. For smaller pillars, surface nu-²¹⁵ 183 cleation of dislocations becomes dominant [23], and the ²¹⁶ 184 rapid stress drop may inhibit correlated surface nucle- 217 185 ation, while for larger pillar size, Taylor-type interaction ²¹⁸ 186 mechanisms prevail [24, 25], and the rapid stress drop ²¹⁹ 187 may suppress cooperative dislocation interactions. 220 188

By contrast, dislocation avalanche under pure stress ²²¹ 189 control is clearly associated with correlated dislocation ²²² 190 motion. According to Eq. 1, when $\alpha = 0$, the stress rate ²²³ 191 cannot sense the internal dislocation activity. Thus, the ²²⁴ 192 stress level keeps almost constant during each avalanche²²⁵ 193 event (see Fig. 3a). If one activated source leads to the ²²⁶ 194 formation of a weaker one, it can be immediately acti-²²⁷ 195 vated. Thus, distinctly different from the strain control 228 196



FIG. 3. Typical simulation results under different loading modes for pillar with d = 1000 b. (a) Stress-strain curves; (bd) Snapshots of dislocation configurations (from top view) at a strain value of 0.4%, arrows indicate the bowing out directions of activated sources

case discussed above, multiple sources can operate in a correlated fashion (see Fig. 3d). All correlated sources contribute then to an increasing magnitude of the strain 199 burst, turning it into an "avalanche". Such highly corre-200 lated dynamical behavior suggests a close-to-criticality nonequilibrium state [3]. 202

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Since it is difficult to experimentally achieve such extreme machine stiffness, it is then interesting to examine dislocation dynamics with finite machine stiff-All the results in Fig. 3a correspond to the ness. same size and initial dislocation configuration. The calculated stress-strain curve with finite machine stiffness $(\alpha = 0.5, \dot{\sigma}_0 = 0)$ in Fig. 3a displays a very similar behavior to experimental results [8, 21], and exhibits a serrated yield character with longer decaying stages as compared to pure strain control. The observation of simultaneous operation of multiple sources in Fig. 3c suggests that a finite machine stiffness actually promotes correlated dislocation motion, compared with pure strain control.

To further elucidate the statistical difference between avalanche versus quasi-periodic dynamics, a simple dislocation based branching model is proposed. It is inspired by the present 3D-DDD simulations, and motivated by Zapperi's sand-pile branching model [26], in which we translate the branching idea into dislocation language. The discrete plastic deformation is assumed to mainly proceed through the intermittent activation of dislocation sources [27, 28]. One activated source may lead to the stochastic generation/activation of other sources, similar to a branching process shown in Fig. 4a.

The detailed algorithm proceeds as follows. Assuming

a pillar initially with n_s dislocation sources, we can randomly give each source a specific length λ according to a given source length probability distribution. The fate of each source (active or not) is determined by checking whether the instantaneous applied stress σ_k can reach the source operation stress,

$$\sigma_k \cdot M \ge \tau_0 + \alpha_1 \mu b \sqrt{\rho} + \alpha_2 \mu b / \lambda \tag{2}$$

where M is Schmid factor, the three terms on the right hand are lattice friction stress, the elastic interaction stress described by Taylor relation, and the source strength, respectively. α_1 and α_2 are dimensionless constant, set to 0.5 and 1 [28], respectively. ρ is the instantaneous dislocation density, estimated by dividing the total source length by the pillar volume.

Once the weakest source is activated during deforma-242 tion, a strain burst begins [28, 29]. After each source 243 is activated, the burst strain S_k increases by a specific 244 value $d\varepsilon^p$. Considering that $\dot{\varepsilon}^p$ is much higher than the 245 applied strain rate $\dot{\varepsilon}_0$ during a strain burst, according 246 to Eq. 1, σ_k drops by $Ed\varepsilon^p \alpha/(\alpha+1)$, and the total 247 strain increases by $d\varepsilon^p/(\alpha+1)$. It is assumed that the 248 activated source is broken (ceases to operate) after it 249 sweeps the entire slip plane once. However, it can ran-250 domly trigger the generation of additional n_a sources. If 251 the newly generated source can be activated according 252 to Eq. 2, it triggers subsequent generation of n_a sources. 253 Otherwise, the new source is stored for possible disloca-254 tion generation, which may activate during subsequent 255 deformation stages. This branching source generation 256 process repeats itself until all dislocation sources cannot 257 be activated under the combined effect of the instanta-258 neous applied stress and the resistance stress, given by ²⁸² 259 the right side of Eq. 2 (see Fig. 4a). At this instance, 283 260 this strain burst event stops and the stress continues to ²⁸⁴ 261 increase till it triggers another strain burst event. 262

In the following, we investigate the slip statistics using ²⁸⁶ 263 this abstract branching model, and compare to the more ²⁸⁷ 264 fundamental DDD simulations discussed above. Com-288 265 pression tests are also modeled for Cu pillars with di-289 266 ameter d=1000 b and 3000 b. Similar to DDD simula- ²⁹⁰ 267 tion, surface nucleation is not considered. If the stress is ²⁹¹ 268 higher than the surface nucleation stress (about 1.2 GPa²⁹² 269 for Cu [30]) or if the strain is higher than 0.5, events ²⁹³ 270 are not recorded. If there is only one activated source, 294 271 each burst strain corresponds to the generated plastic 295 272 strain when the dislocation sweeps the entire slip plane ²⁹⁶ 273 once. Therefore, $d\varepsilon^p$ is set to $bM/H/\cos\beta$ [28], where ²⁹⁷ 274 β is the angle between the normal direction of the slip ²⁹⁸ 275 plane and the loading orientation. Through examination 299 276 of the dislocation configuration evolution, n_a is taken as $_{300}$ 277 the nearest integer of $2 \cdot rand$, where rand represents a $_{301}$ 278 random value from 0 to 1. Accordingly, the probabilities 302 279 of n_a being 0, 1 and 2 are 25%, 50% and 25%, respec- 303 280 tively. This is different from previous sand-pile branch- 304 281



FIG. 4. (a) Schematic showing the random branching dislocation source generation and activation process, n_a is the number of newly generated dislocation sources, green filled circles represent that new source is activated, only activated source may trigger further branching process; (b-d) Typical predicted results for pillar with d = 1000 b, (b) Stress-strain curve, (c) Comparison of activated source number during each burst under pure strain control, (d) Probability density function of burst displacement for different machine stiffness; (e) Probability density function of burst displacement for different sample sizes

ing model [26], where the new activated site number was taken a constant value of 2. $n_a = 0$ means that the source is destroyed after operation once, $n_a = 1, 2$ indicate that other sources are generated due to interactions with other dislocations, cross slip, forming superjogs, or forming dipolar loops [7]. Note that, more deactivated sources may be left in the sample if $n_a=2$, leading to a slight increase in the dislocation density ρ after each branching process. This results in an increase in the elastic interaction resistance stress. Similar to 2D-DDD simulations [31], the source length is assumed to follow a Gaussian distribution, with a mean value $\overline{\lambda} = d/2$, determined according to the yield stress of our DDD results. Its standard deviation is set to $20\%\lambda$, so that the predicted activated source number for each strain burst event is statistically equivalent to those obtained by our DDD results under pure strain control (see Fig. 4c).

Fig. 4b presents predicted typical stress-strain curves under different loading modes, which agree well with our simulation results in Fig. 3a, including the stress level and the stepped or serrated burst features. In addition, the power law scaling of burst displacement ΔU is also well reproduced under pure stress control for different pillar sizes in Fig. 4e. The power law exponent of the $_{360}$ probability distribution of ΔU agrees with that obtained $_{361}$ by the present 3D-DDD. Fig. 4d clearly indicates that $_{362}^{363}$ gradually become too wide to recognize proper scale-free power law statistics. $_{366}^{364}$

The excellent agreement between the abstract branch-367 311 ing model prediction and the fundamental 3D-DDD sim- 368 312 ulations further verify that hard machine stiffness leads 369 313 370 to deviation from scale-free SOC, because the rapid 314 371 stress relaxation disturbs correlated dislocation motion. 315 372 The current finding offers a new pathway towards con- $\frac{373}{373}$ 316 trolling the correlated extent of dislocation dynamics 374 317 and the intermittent statistics by tuning the machine 375 318 stiffness. It opens up new possibilities for novel ex- 376 319 periments with faster response rate that can reveal the ³⁷⁷ 320 quasi-periodic oscillation dynamics of dislocation sys-378 321 tems. The importance of often-neglected interaction 322 with the external loading system on intermittent plastic 323 381 flow has been demonstrated. The complex dynamics of 324 382 collective dislocations producing strain bursts is shown 383 325 to be controlled through simple tuning of the relative ³⁸⁴ 326 value of driving force rate to internal relaxation rate. 327

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