Power-Law Statistics for Avalanches in a Martensitic Transformation

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We devise a two-dimensional model that mimics the recently observed power-law distributions for the amplitudes and durations of the acoustic emission signals observed during martensitic transformation [Vives et al., Phys. Rev. Lett. 72, 1694 (1994)]. We include a threshold mechanism, long-range interaction between the transformed domains, inertial effects, and dissipation arising due to the motion of the interface. The model exhibits thermal hysteresis and, more importantly, it shows that the energy is released in the form of avalanches with power-law distributions for their amplitudes and durations. Computer simulations also reveal morphological features similar to those observed in real systems.

Many spatially extended driven systems naturally evolve to a marginally stable state characterized by avalanches with power-law distributions for their amplitudes and durations reflecting lack of intrinsic length scales and time scales in the system. Such a state is termed as a self-organized critical (SOC) state by Bak et al. [1]. Several physical systems exhibit SOC features: for example, earthquakes [2], acoustic emission from volcanic rocks [3], and stress drops during jerky flow [4], to name a few. Recently, Vives et al. [5], measured the acoustic emission (AE) signals during martensitic transformation of Cu-Zn-Al single crystals under thermal cycling. They reported power-law statistics for the amplitudes and durations of the AE signals during both cooling and heating runs. To the best of our knowledge, there is no strain (or displacement) based model of martensitic transformation which explains these results. Moreover, any prospective model has to take into account the nonequilibrium nature of the hysteresis. Even though extensive theoretical studies exist on martensitic transformations [6–8], the influence of dissipation and defects on hysteresis has received very little attention. Here, we propose a simple phenomenological model which captures the power-law distribution of AE signals along with the thermal hysteresis of the transformation. Below, we will briefly collect SOC-type features of the martensitic transformation relevant for modeling the system.

Martensitic transformation is a first-order, solid-solid, diffusionless, structural phase transition. On cooling, the unit cell gets distorted [6–8], leading to the nucleation of thin platelike product domains with a twinned structure. This induces internal strains, which in turn induce long-range fields that block the transformation leaving the system in a two phase metastable state. (Note that this implies the existence of a built-in threshold mechanism.) Thus, the amount of the transformed phase is entirely determined by the excess free energy, and an additional undercooling is required for further growth. This implies that thermal fluctuations have little role in the transformation kinetics. Thus, the transformation is athermal and hence the nucleation is athermal, usually occurring at defects such as dislocations [6–8,10]. Further, the emission of acoustic energy in the form of bursts implies that inertial effects are important. Indeed, Bales and Gooding, and later Reid and Gooding, [11] studied the importance of including the inertial effects. Vives et al. attribute the mechanism of irreversible release of the elastic energy in the form of avalanches, each of which correspond to the motion of one (or more) interface, to the evolution of the system from one metastable state to another [5]. Since the interface moves at near velocity of sound, there is dissipation associated with it. We include all these features along with the long-range interaction between the transformed domains.

We consider, a 2D square-to-rectangle transition, for which the free energy is usually a function of all three components of strain defined by $e_1 = (\eta_{xx} + \eta_{yy})/\sqrt{2}$, $e_2 = (\eta_{xx} - \eta_{yy})/\sqrt{2}$, and $e_3 = \eta_{xy} = \eta_{yx}$, where $\eta_{ij} = -\frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})$ refers to the components of the strain tensor and $u_i$ is the displacement field in the direction $i$ ($i = x, y$). Here, $e_1$ is the bulk dilatational strain, $e_2$ is the deviatoric strain, and $e_3$ is the shear strain. In athermal martensites, deviatoric shear strains play a dominant role in the transformation kinetics [6]. Thus, we consider the deviatoric strain $e_2 = e(\vec{r})$ as the principal order parameter since volume changes are small [6–8,12]. The effect of other strain components $e_1$ and $e_3$, i.e., the bulk and shear strain, is accounted phenomenologically by considering a long-range interaction between the deviatoric strains.

We write the rescaled free-energy functional as 
$$F[e(\vec{r})] = F_L[e(\vec{r})] + F_{1r}[e(\vec{r})],$$
where $F_L$ is
$$F_L = \int d\vec{r} \left[ f_1[e(\vec{r})] + \frac{D}{2} [\nabla e(\vec{r})]^2 - \sigma(\vec{r})e(\vec{r}) \right],$$
(1)
where $D$ and $\sigma$ are in a scaled form. $F_{1r}$ is an effective long-range term that describes transformation induced strain-strain interactions. In Eq. (1), $f_1[e(\vec{r})] = \frac{\delta^2 F}{\delta e^2}(\vec{r})^2 - \frac{1}{2} \varepsilon(\vec{r})^2 + \frac{1}{2} \varepsilon(\vec{r})^2$ is the usual Landau polynomial for a
first-order transition, where $\delta T = (T - T_0)/(T_0 - T_c)$ is the scaled temperature. $T_0$ is the first-order transition temperature at which the free energy for the product and parent phases are equal, and $T_c$ is the temperature below which there are only two degenerate global minima $e = \pm e_M$. Following Cao et al. [10], the effect of localized defects acting as nucleation sites is simulated by an inhomogeneous stress field, $\sigma(\vec{r})$. This term modifies the free energy $f_j$ in a way that renders the austenite phase locally unstable, leading to the nucleation of the product phase. As mentioned earlier, the physical cause of the long-range interaction is the coherency strain between the parent and the product phases. Such an interaction is also expected to arise due to the coupling of the austenite-martensite phases, the authors introduce the cutoff distance $\Delta t = 0.2$. We studied both the single defect and many defect nucleation case. Here, we report results on the multisite case and only mention results on the single site case wherever necessary.

Consider the nucleation and growth for a single quench. We use a random distribution of defects and represent their stress field by $\sigma(\vec{r}) = \sum_{j=1}^{j_{\text{max}}} \sigma_0(\vec{r}_j) \exp[-(|\vec{r} - \vec{r}_j|^2)/\xi^2]$, where $\vec{r}_j$ refers to the scaled coordinates of the defect sites and $j_{\text{max}}$ is the total number of defect sites. $\sigma_0(\vec{r}_j)$ is taken to be uniformly distributed in the interval $[-0.3, 0.3]$. Initially, the system is taken to be in a homogeneous state with $\epsilon(\vec{r}, 0)$ distributed uniformly in the interval $[-0.005, 0.005]$. At $t = 0$, we switch on the stress field $\sigma(\vec{r})$. Figure 1 shows snapshots of the transformation at $t = 10, 12, 15,$ and $50$. (Grey regions represent the austenitic phase $\epsilon = 0$, and black and white regions represent the two variants.) Nucleation of the product phase occurs with a value $\epsilon \sim \pm 2$ at several locations, where the magnitude of the stress field is sufficient to make the system locally unstable ($t = 10$). We note here that the value of $\epsilon$ for the two variants is larger than that given by $f_j[\epsilon(\vec{r})]$ alone ($\epsilon_M \sim \pm 1.31$ for these parameters) due to the long-range interaction. In a short time, we see the other variant being created adjacent to these nuclei. By $t = 12$ (Fig. 1), the structure further develops into twinned arrays, propagating along [111] and [111] directions. We also see that several new domains are nucleated at a finite distance from the preexisting domains which is consistent with the autocatalytic nucleation mechanism known to operate.
in martensitic transformation [8,9]. Although the new nucleation sites most often coincide with the defect sites, occasionally they are seen in defect-free regions. (Similar observation was made in the single site case also.) This can be attributed to the stress accumulation at these sites as a result of the long-range term due to the preexisting martensitic domains. Note that the twinning is irregular which is again due to the mutual interaction between the various domains. There is very little growth beyond \( t = 30 \). Thin needlelike structures can also be seen to emerge from larger domains \( t = 50 \) as reported by Vives et al. [5]. There is also a distribution of domain sizes.

We simulate thermal cycling of the transformation by continuously changing \( \delta T \) from +40 to −80 and back, in a duration of \( t = 1000 \) units at a constant rate, for both the heating and the cooling runs. For the reverse cycle, the final configuration of the cooling run is used as the initial configuration. Figure 2 shows the area fraction \( \phi_A \) versus \( \delta T \) for the cooling and heating runs (○). In the cooling run, the transformation starts with a rapid increase in \( \phi_A \) at about \( \delta T_{ms} \sim -2.0 \), and is completed by \( \delta T_{mf} \sim -59 \). In the heating run, the parent phase appears only at \( \delta T_{as} \sim -26.0 \) and \( \phi_A \) decreases almost linearly till the transformation is nearly complete at about \( \delta T_{af} \sim 18 \). [For the sake of comparison, we have also shown the single site hysteresis loop by (●).]

The most important feature of the model is that the changes in \( \phi_A \) are actually jerky which can only be seen on a finer scale. Since the rate of energy dissipated \( dE/dt = -2R(\delta t) \), we calculated \( R(\delta t) \) [or \( R(\delta T) \)]. In Fig. 3, we plotted \( R(\delta T) \) with the inset showing the enlarged section of the peak which clearly shows that the rate of energy release occurs in bursts consistent with the acoustic emission studies [5]. (Latent heat also shows a pattern similar to Fig. 3 [17].) Further, the distribution of the amplitudes of \( R(\delta t) \) denoted by \( R_A \) has a tendency to approach a power-law \( D_R(R_A) \sim R_A^{-\alpha_R} \) with \( \alpha_R \sim 2.6 \) [○] in Fig. 4. We have also shown the single site results by (●).] Similarly, the distribution \( D_R(\Delta t) \) of the durations \( \Delta t \) of the energy bursts scales with \( \Delta t \) given by \( D_R(\Delta t) \sim \Delta t^{-\tau_R} \) with \( \tau_R \sim 3.2 \). Although the scaling regime is almost identical to \( D_R(R_A) \), we find that the scatter is slightly more in this case. (This is true of experimental results as well [5] and in SOC models [1].) The conditional average [18] of \( R_A \) for a given \( \Delta t \) denoted by \( \langle R_A \rangle_c \) behaves as \( \langle R_A \rangle_c \sim \Delta t^{\nu} \). We get the exponent value \( \nu_R \sim 1.36 \). We also find that the scaling relation \( \tau_R = x_R(\alpha_R - 1) + 1 \) is satisfied quite well. In experiments, however, one measures the amplitude of the AE signals \( A_{AE} \), i.e., \( R_A \sim A_{AE}^2 \). Using the relationship between the two joint probability distributions \( D(R_A, \Delta t) \propto D(A_{AE}, \Delta t)/A_{AE} \), it can be easily shown that \( \alpha_R = (\alpha_{AE} + 1)/2 \), where \( \alpha_{AE} \) is the exponent corresponding to \( A_{AE} \). The other two exponents remain unchanged. Using the experimental values [5] \( \alpha_{AE} \sim 3.8 \) , \( \tau_{AE} \sim 3.6 \), and \( x_{AE} \sim 1 \), we see that \( \alpha_R \sim 2.4 \). Thus, we see that our values are in reasonable agreement with experiments, considering the fact that real systems are 3D. It must be stated here that in 3D even the number of variants are generally more, and one also expects that the
The presence of defect sites only triggers the initial nucleation process. This must be contrasted with disorder based Ising models [19] which also produce power-law statistics for avalanches and field induced hysteresis. However, by subjecting the samples to repeated thermal cycling, Vives et al. have verified that, in martensite transformation, it is the dynamical (transformation induced) disorder that is at the root of the avalanches. In this sense, our model is the first to capture both the thermal hysteresis and the jerky nature of the transformation based on dynamical disorder and is independent of quenched disorder.

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