Microstructural heterogeneity and dynamic shear localization

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Dynamic shear localization attracted interest as both experimental and theoretical evidence suggested that its origins are not only due, as believed, to thermal softening, but are most likely related to microstructural evolutions, the latter being driven by a critical value of the stored strain energy. Yet, nothing is known about the effects of the distribution (heterogeneity) of this stored energy at the microstructural level. Using the well-known concept of Shannon's entropy, we systematically compare different heterogeneities, and conclude that small amounts of microstructural heterogeneity may significantly influence shear localization, as opposed to larger values of homogeneously distributed strain energy. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4767654]

A major dynamic deformation and failure mechanism of crystalline solids consists of abrupt localization of the plastic deformation into narrow zones, referred to as adiabatic shear bands (ASBs). The term *adiabatic* implies that heat transfer over short temporal and spatial length scales is negligible, as was reported by Tresca.[1] Zener and Hollomon[2] proposed that the inherent temperature rise causes material softening, which may overcome the strain hardening effect, ultimately leading to strain localization. More recently, Rittel *et al.*[3] proposed that the stored energy of cold work,[4] namely the part of the invested mechanical work that is not dissipated into heat,[5] causes microstructural re-arrangements (dislocations' configuration) whose most obvious manifestation is the formation of new nano-sized grains by dynamic recrystallization (DRX[6]). These authors proposed that the dynamically recrystallized grains cause local softening of the surrounding hardened matrix material, thereby providing the necessary perturbation whose growth is the shear band itself. Considering the additional deformation micro-mechanism of twinning present in many materials, Osovski *et al.*[7] proposed a numerical model illustrating the competition between dislocation-mediated plasticity (DRX) and twinning, these mechanisms being introduced into a finite element (FE) model. This model was subsequently expanded to include a full thermomechanically coupled scheme.[8]

Yet, while the onset and subsequent evolution of the shear localization process can be evaluated *qualitatively* from typical simulation results, a more *quantitative* and systematic way to evaluate those issues is still missing. A second central issue is that of the role of microstructural heterogeneity on the onset of the shear localization process. Namely, while a macroscopic critical value of the stored energy of cold work was identified as the trigger for shear localization, no information is available so far on the influence of the *distribution* of this energy among various grains, referred to as microstructural heterogeneity in this work. Such heterogeneity is most likely to exist and develop in a polycrystal, where a homogeneous distribution of strain energy would be most likely unphysical.[9] In this paper, we propose to apply the well-known concept of Shannon's entropy,[10] coming from information theory, where it is defined as a measure for the loss of information when calculating the expected value of a random variable. Shannon's entropy is applied here to the characterization of the extent of strain localization throughout the dynamic deformation process. In the present context, the random variable is considered to be the strain at Gauss points, and thus Shannon's entropy can be interpreted as a quantitative evaluation of the number of occupied strain states of a system. If one considers, for instance, the distribution of plastic strain among various grains of a material, as done in the sequel, Shannon's entropy can be calculated to assess the level of order (homogeneity or lack) of and its evolution for this system. For an ordered (homogeneous) distribution, the expectation value (mean plastic strain) contains most of the information, and thus the value of Shannon's entropy is small. However, when a localized band (large heterogeneity in the strain state) is present, the expectation value will smear out its presence, so that a large part of the information will be lost, resulting in high values of the Shannon's entropy. Therefore, using this tool, one can systematically explore the role of the microstructural heterogeneity in a quantitative and thus comparative way, in the context of the evolution of local plastic strains leading to the onset of a shear localization process.

The FE model of a dynamically deforming crystalline solid (including slip and twinning),[7,8] was used, in which each finite element represents a material grain (representative volume element). The model was modified to account for the latent heat resulting from the DRX process as well as the thermo-mechanical coupling effect leading to (linear) material softening.[8] We consider here a square plate under dynamic loading conditions (prescribed velocity in the Y-direction, and plane strain deformation), shown in Fig 1(a). The plate was meshed with a 100×100 C3DR elements structured mesh where each element is $100\,\mu m \times 100\,\mu m \times 100\,\mu m$. All the simulations were carried out using ABAQUS, a commercial FE solver.[11] To study the effect of initial heterogeneity, the latter being understood here as the initial amount of stored energy of cold work per grain, the initial energy values randomly

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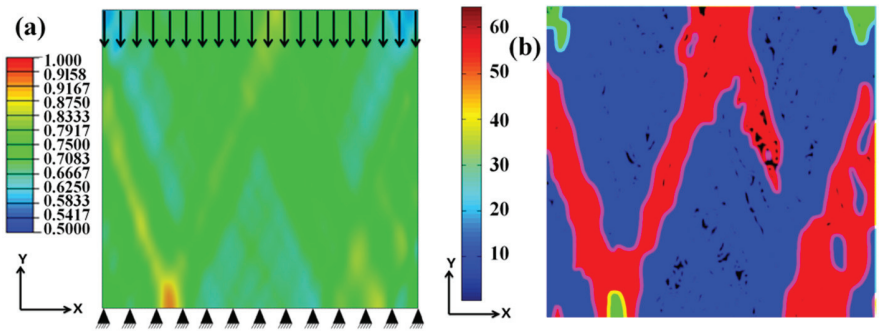

FIG. 1. Model of the plate undergoing dynamic compression. (a) Boundary conditions of prescribed velocity as well as the plastic strain map, projected onto the un-deformed configuration. (b) The corresponding local Shannon's entropies defined on a 9×9 pixel local grid. Note the delineation of the localization bands resulting from application of Shannon's entropy.

sampled from a half-Gaussian, zero-centered, distribution were randomly assigned to each element. The so-called measure of heterogeneity was controlled by systematically varying the standard deviation (STD) of the distribution while limiting the maximal normalized energy level to 1, the latter being the critical value of the stored energy that triggers dynamic recrystallization (E_{DRX}). This latter quantity is determined experimentally, as reported by Rittel *et al.*[3] Elements with an initial value of stored energy will tend to start forming DRX, and thus weaken the material at earlier stages of the deformation process. For clarity, from this point on, all further measures of energy to be used are reported as normalized quantities with respect to E_{DRX}. The STD values that were examined were STD = [0.05 0.1 0.15 0.175 0.2 0.25 0.3 0.4 0.5 0.6 0.75 0.9 1]. For each value of the STD considered, the response of the dynamically loaded plate was simulated, and each simulation was repeated ten times to account for the effect of different random initial spatial distributions. Here, it is important to emphasize that the microstructure of the material is allowed to evolve with strain, irrespective of its initial heterogeneity, as in Refs. 7 and 8. This includes of course the simulations of initially homogeneous material. The simulations' results where then analyzed as follows:

A map of the plastic strain distribution in the plate at selected time intervals was projected onto the un-deformed geometry (Fig 1(a)). For each figure, we calculated the histogram of the plastic strains and used it to calculate the global Shannon's entropy according to Eq. (1).

$$S = -\sum_i \rho_i \ln \rho_i. \tag{1}$$

Here, ρ_i is the probability of finding an element deformed to a plastic strain level of ε_i. The same procedure was then used to obtain for each element a local estimate of Shannon's entropy by calculating the distribution of plastic strain in its neighborhood, which was defined here as the 9×9 pixels (elements) surrounding it. An example of the results of this procedure is shown in Fig. 1(b). This procedure is quite efficient in revealing the location and extent of the localization process for each strain map.

The global Shannon's entropies, calculated for each simulation, were then plotted as a function of the imposed true strain in the Y direction (Fig. 2). One can see that all the cases exhibit a similar behavior in which the entropy first increases with the strain until it reaches a plateau, this point corresponding to a state of dynamic force equilibrium on the plate. From this point on, the entropy starts to decrease indicating that the plastic strain distribution in the equilibrated specimen is becoming more uniform, meaning a smaller number of occupied strain states. However, at some point in time, the Shannon's entropy reaches a local minimum (arrowed in Fig. 2), immediately followed by a rapid increase. This inflexion point can be considered as the onset of the shear localization, as it indicates a localized concentration of strain of the kind shown in Fig. 1. Note that results are presented here for a maximum STD of 0.4. While greater values were analyzed, it appears that the number of elements having an initial energy level of 1 is non-negligible, thus causing almost immediate localization, which is of little interest to the present work. In Fig. 3, we present a plot of the strain as a function of the standard deviation of the initial energy at which the entropy reaches a local minimum (inflexion point, arrowed in Fig. (2)). Fig. 3 leads to the following two observations:

(1) Increasing the material heterogeneity (STD) leads to early initiation of the localization process, eventually followed by earlier macroscopic failure. Note that throughout this work, we did not examine nor include a failure criterion (e.g., critical strain) in the numerical model.

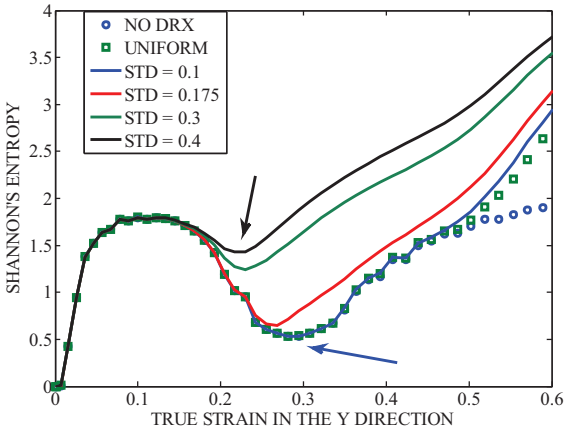

FIG. 2. The evolution of Shannon's entropy with imposed strain in the Y direction. Circles represent a simulation in which DRX cannot happen; squares are for a simulation in which no initial energy was distributed. The rest of the lines stand for simulations in which an initial amount of stored energy was randomly distributed between the elements by sampling from a Gaussian distribution with different standard deviation values (0.1, 0.175, 0.3, and 0.4). The arrows indicate the local minima from which the entropy grows rapidly, indicating the onset of localization.

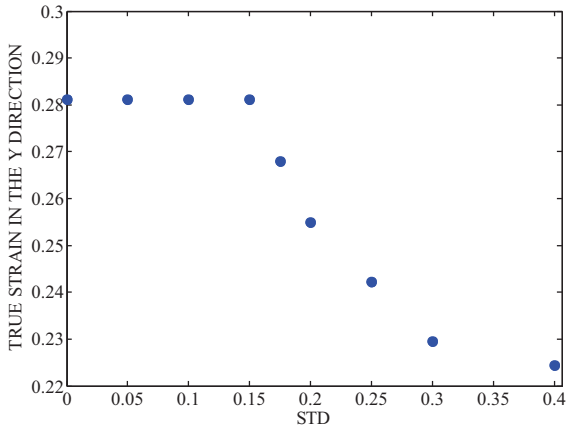

FIG. 3. Plastic strain value corresponding to the local minima in Shannon's entropy (onset of localization) vs. STD of the different initial distributions of energy. Mean values are calculated for five runs of STD values.

(2) There exists a region in the STD domain, between 0.15 and 0.4, in which the response of the material to a change in its energy content and distribution is very pronounced. Such an abrupt change is reminiscent of a percolation loss of stiffness,[12] even if at the present stage, additional work is needed to confirm this observation.

One may now wonder about the dominant factor that precipitates localization, namely *initial heterogeneity* and/or *high initial energy content* in the specimen.

To answer this question, we calculated the average amount of energy per element in a plate for which the STD was taken to be 0.3. Note that from Fig. 3, this level of STD corresponds to early localization in the plate. The energy was calculated by integrating the Gaussian distribution with this STD and dividing the obtained result by the number of elements in the plate, yielding the value of $E_{AVG} = 0.12$. The same total amount of energy was then distributed *uniformly* among all the elements for the simulation. We then further increased the averaged initial amount of energy in each element (E_{AVG}) up to a value of STD = 0.4, by considering larger STD values. Fig. 4(a) presents a comparison of the heterogeneous case (STD = 0.3) for which $E_{AVG} = 0.12$, with the uniform cases in which $E_{AVG} = 0.15$, 0.3, and 0.4. It appears that even with the highest value of initial energy used ($E_{AVG} = 0.4$), which is more than twice the total amount of energy than in the normally distributed case presented at the same graph (STD = 0.3 and $E_{AVG} = 0.12$), the localization is observed to initiate at a larger imposed strain than in the less energetic heterogeneous case. This indicates that heterogeneity in itself (i.e., the existence of a small amount of sites with high values of initial energy) plays a key role in initiating the localization process.

To further refine this observation, we ran a series of simulations in which the initial energy for each element was sampled as before. Each element whose normalized energy was smaller than a prescribed value (E_C in the range 0.3-0.6) was pre-assigned a zero initial energy. Each simulation was repeated five times. The goal of those simulations was to explore the role of the *tail of the Gaussian distribution* (standard deviation, i.e., heterogeneity). Fig. 4(b) shows the Shannon's entropy for those various cases as a function of the prescribed longitudinal strain in the plate. It is interesting to compare the imposed strain at which localization starts for those cases where only the tail of the distribution was retained with the full distribution and the zero initial energy one. One can note from Fig. 4(b) that this strain, irrespective of the remaining tail of the distribution, is always smaller than its counterpart obtained from a simulation in which no initial energy was prescribed. Those results confirm that the presence of a strong heterogeneity, even in small amounts, has a drastic effect to a much stronger extent than a high, yet homogeneous, level of initial energy.

We have shown in this paper that Shannon's entropy is a powerful quantitative tool to characterize strain heterogeneity, thus localization. Such a tool is particularly useful to quantitatively analyze results of numerical simulations (and future experimental results) in terms of onset and strength of the localization process. This study has allowed us to gain insight on the nature of the thermodynamic driving force

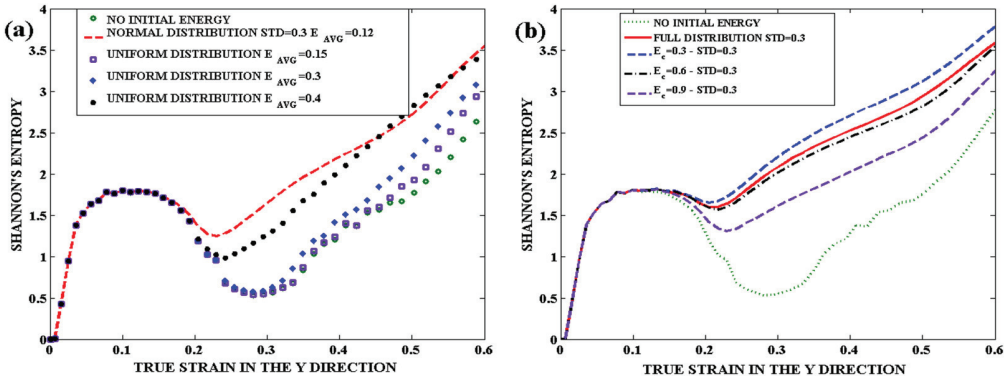

FIG. 4. A comparison of the evolution of Shannon's entropy with the imposed strain in Y direction. (a) The effect of overall averaged energy per element by comparing a simulation with normal distribution of energies (STD = 0.3) corresponding to an average value of E_{AVG} 0.12 and 3 cases in which the same initial energy was assigned to all elements uniformly. Note that for initial values of E_{AVG} of up to 0.4, the localization starts earlier than in the normally distributed cases. (b) The effect of the normal distribution's tail is studied by zeroing all initial energy values smaller than $E_C = (0.4, 0.5, 0.6)$ with STD = 0.3, and comparing the result with the full distribution with the same STD (0.3). One can note that by removing energy from the system while keeping a small amount of highly energetic elements, the beginning of localization process is hardly effected.

leading to localization, i.e., dynamic recrystallization. We have shown that the dominant factor in the process is the distribution of this stored energy (driving force) among grains, namely its heterogeneity as characterized by its standard deviation. When the latter is systematically varied, a percolation-like phenomenon in the macroscopic localization strain is observed. In that context, one should mention the work of Bigoni and Capuani[13] who observed similar localization patterns upon introduction of a perturbation to an equilibrated strain field. We also showed that the stronger the heterogeneity, the earlier localization will occur, with a much stronger effect than that of a homogeneously distributed level of (high) energy. Those results refine the concept of a critical level of stored energy of cold work as a driving force for strain localization, emphasizing the importance of its *distribution* whose integral is the above-mentioned level of stored energy of cold work.

The proposed approach is of a general character, in the sense that strain heterogeneity exists in single and multiphase materials alike, as evidenced recently by grain-scale studies using a combined grid method and infrared thermography.[9]

The present results are expected to provide new guidelines for further experimental characterization of dynamic strain localization phenomena and future material design.

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