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R. E. Rudd, E. T. Seppala, L. M. Dupuy, J. Belak

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R. E. Rudd, E. T. Seppälä*, L. M. Dupuy, J. Belak
Lawrence Livermore National Laboratory
University of California, L-045
Livermore, CA 94551-0808 USA

ABSTRACT

Simulation of ductile fracture at the atomic scale reveals many aspects of the fracture process including specific mechanisms associated with void nucleation and growth as a precursor to fracture and the plastic deformation of the material surrounding the voids and cracks. Recently we have studied void coalescence in ductile metals using large-scale atomistic and continuum simulations. Here we review that work and present some related investigations. The atomistic simulations involve three-dimensional strain-controlled multi-million atom molecular dynamics simulations of copper. The correlated growth of two voids during the coalescence process leading to fracture is investigated, both in terms of its onset and the ensuing dynamical interactions. Void interactions are quantified through the rate of reduction of the distance between the voids, through the correlated directional growth of the voids, and through correlated shape evolution of the voids. The critical inter-void ligament distance marking the onset of coalescence is shown to be approximately one void radius based on the quantification measurements used, independent of the initial separation distance between the voids and the strain-rate of the expansion of the system. No pronounced shear flow is found in the coalescence process. We also discuss a technique for optimizing the calculation of fine-scale information on the fly for use in a coarse-scale simulation, and discuss the specific case of a fine-scale model that calculates void growth explicitly feeding into a coarse-scale mechanics model to study damage localization.

Keywords: void growth, void coalescence, molecular dynamics, multiscale modeling, adaptive sampling

Introduction

The behavior of many solid systems of interest today is governed by physics on multiple length scales, and a particularly important example is the fracture of ductile solids. In the process of ductile fracture, voids nucleate, grow and coalesce, and it is this linking process that creates the fracture. [1] Voids nucleate from weak points in the material such as inclusions and grain boundary junctions. They grow, reducing the tensile stress in the material and the associated elastic energy. The material

surrounding the void must deform plastically in order for the void to grow appreciably. Ultimately, the voids link to form the fracture surface, which exhibits remnants of the voids in the dimpled surface characteristic of ductile fracture.

Of particular interest to us is dynamic fracture; i.e., fracture at high strain rates such as found in the release wave that is created when a compressive shock wave reflects from a free surface or interface. [2] The resulting ductile fracture process may involve the nucleation and growth of voids throughout an extensive region of the system, prior to the formation of any well-defined fracture. As these voids grow and link up they may cause a scab of material to be detached and ejected in a process known as spallation. At high strain rates slow processes such as diffusion are irrelevant, and molecular dynamics (MD) has the ability to capture the relevant physics.

Ductile fracture has typically been modeled at the continuum level, in a variety of models that may or may not model voids explicitly. Seminal work in this area includes the work of McClintock [3], Rice and Tracey [4] and Gurson [5]. Void-based models of spallation include the DFRACT model [2], the spall model of Cochran and Banner [6], and the model of Tonks and coworkers [7]. There has been extensive work in modeling ductile fracture at the continuum level, and these references are by no means exhaustive.

We have undertaken an extensive study of void processes at the atomistic level [8-12]. Here we review some of the more recent work examining the effect of strain-rate triaxiality on void growth [13] and an extensive series of simulations of the coalescence process [14-15]. Large-scale atomistic models provide detailed information on void interactions and the plasticity generated as voids coalesce, based solely on the constitutive properties inherent in the interatomic forces. The details of the plasticity may then be used to inform dislocation dynamics and continuum plasticity models in order to develop models that scale beyond the nanoscale.

Methods

We have conducted large-scale molecular dynamics simulations of void nucleation, growth and coalescence. The same basic techniques were used to conduct the simulation in each case. Following the approach of Belak [8], a collection of atoms in a representative volume element of the solid is positioned in a three-dimensional simulation box with periodic boundary conditions. These atoms may be in a single crystal or a polycrystal [8,9]. The dynamic trajectories of the atoms are calculated by integrating Newton's equations of motion (F=ma) using an explicit time integrator with a fixed time step, e.g. a time step of 6.7 fs for EAM copper (see Ref. [13] for the details). The system is brought to thermal and mechanical equilibrium at the desired initial temperature through the use of a thermostat and through changing the box volume to eliminate any stresses.

Once the system is equilibrated, the thermostat is turned off for the ensuing simulation. At this point the atoms in one or more regions of the system may be removed, creating cavities that simulate very weakly bound inclusions that are preferential nucleation sites for voids. In this case the material comprising the inclusion is assumed to play no role in the void growth process once the void has nucleated, and the debonding process is assumed to be sufficiently rapid that the details are unimportant. This debonding process is the subject of on-going investigation. Starting with the thermalized initial state, the simulation box is expanded at a specified strain rate, using the technique of Parrinello and Rahman. [16] The expansion may be perfectly triaxial, such that the box is expanded equally in all three dimensions, or it may be uniaxial as in a shock wave, or it may involve some other state of strain. Note that strain controlled simulations are stable under void growth, so that as the void grows, the magnitude of the mean tensile stress decreases and the tendency for further void growth is reduced; by contrast stress-controlled simulations may be unstable since as the void grows the material may be less able to support tensile stress and hence the void would grow faster. Since no thermostat is used in our simulations during the expansion, the temperature changes, but not greatly. During the initial elastic expansion, the system undergoes adiabatic cooling. Once plastic deformation begins, mechanical energy is dissipated through dislocation motion and the system heats up. In a typical simulation reported here, the system starts at room temperature (300K) drops to 250K during the elastic phase, and rises to roughly 600K. The final temperature is well below the melting point and no other phase transformation takes place.

During the course of the simulation, many properties of the system are monitored. In addition to the temperature already mentioned, the stress and the potential and kinetic energies are calculated. The full stress tensor is computed using the virial formula:

$$\sigma_{\alpha\beta} = -\frac{1}{V}\left(\sum_i p_{i\alpha} p_{i\beta} / m_i + \sum_i \sum_{j>i} r_{ij\alpha} f_{ij\beta} \right) \quad (1)$$

where

$p_{i\alpha}$ = momentum of the i^{th} atom in the α direction

m_i = mass of the i^{th} atom

$r_{ij\alpha}$ = distance to the j^{th} atom from the i^{th} atom in the direction α

$f_{ij\alpha}$ = force on the j^{th} atom from the i^{th} atom in the direction α

and V is the system volume (for a recent discussion of atomistic stress see Ref. [17]). Of particular interest in the study of void growth is the mean stress σ_m = Tr σ/3 and the von Mises stress $\sigma_e = [(3/2)\ \mathrm{Tr}\ (\sigma')^2]^{1/2}$ where $\sigma'_{\alpha\beta}$ is the deviatoric stress. We also calculate the stress triaxiality $\chi = \sigma_m / \sigma_e$.

In addition more recently the void growth and plastic deformation in the system have been quantified in various ways. The void surface atoms are identified and the void surface is triangulated [13,18]. The triangulation is constructed on the fly distributed across the domain decomposition of the parallel computation using an advancing front technique to find a close analog of the r-reduced surface used for visualization of biological molecules. [18] The triangulation of the surface is then used to calculate the void volume, surface area and multipole moments that quantify the void shape. We also identify atoms in dislocation cores and compute the dislocation density and the Burgers vectors of the dislocations (see Figure 1).

[Fig. 1]

We have studied void processes related to fracture in a variety of materials including copper, aluminum, tantalum, molybdenum and iron. The results we focus on here are from simulation of copper using the embedded atom method (EAM) interatomic potential due to Oh and Johnson. [19] A parallel molecular dynamics code, MD3D, that has demonstrated good scaling to 256 CPUs was used for the copper void studies. [13-15]

Growth of a Single Void

We have used the atomistic simulations to model the nucleation, growth and coalescence of voids during ductile fracture at high strain rates. The nucleation studies were done some time ago [8,9] and we will not describe them further here. Void growth has been studied in single crystal and polycrystal systems. Here we focus on the single-crystal studies in which nucleation from an inclusion was simulated, as described above, by introducing a cavity just as the expansion of the simulation box began. These simulations consist of about 1 million copper atoms in cubic boxes that are typically 22 nm on a side. The initial void radius is typically 1/10 of the box size. Regardless of the strain rate and the triaxiality of the expansion, the same general sequence of events was observed in copper. Initially, the system expanded elastically, as seen in Figure 2 up to a strain of 5.2%. No dislocations or secondary voids were nucleated during this period of the simulation. The size and shape of the void changed roughly in accordance with the changes to the simulation box; for example, if the box expanded uniaxially, then the void became elongated in the direction of the expansion. In the second phase of the expansion, dislocations began to nucleate at the void surface. In particular, 1/6<211> partial dislocations nucleated on the {111} glide systems as expected. During triaxial expansion of a system containing a spherical nucleus, the symmetry of the system would lead one to expect that all 12 glide systems would be equally activated, and the activity was observed to be roughly equal. The small amount of symmetry breaking can be attributed to thermal fluctuations, and indeed it is observed to be dependent on the temperature and strain rate. During uniaxial expansion, the dislocation activity is biased by the applied shear stress, and the glide systems are not equally active. Ultimately, full dislocation loops detach from the void surface and propagate away, as can be seen in Figure 1 [10]. Dislocations emitted from the surface leave steps, albeit less defined than on a flat surface, effecting an expansion of the void. This void growth acts to relieve the mean tensile stress, so the stress plateaus and ultimately drops as

seen for example in Figure 2 [13]. Other aspects of dislocation emission from voids have been analyzed in a recent article. [20]

[Fig. 2]

The sequence of events in void growth due to uniaxial expansion is particularly interesting, as shown in Figure 3. Following the initial elastic phase in which the void elongates, becoming prolate in the direction of the expansion, plasticity begins and the bias due to the applied shear stress favors dislocation nucleation from the equator of the void. The result is that the void grows transversely to the expansion and undergoes a prolate-to-oblate transition [13]. We have used multipole moments to quantify this shape change. It has been observed previously in two-dimensional continuum modeling of void growth in which the transition was quantified by the log of the ratio of the major to minor axis lengths [21]; in our 3D simulations with no rotational symmetry axis (due to the crystal lattice), the quadrupole moment is a well defined means of quantifying the eccentricity of the pseudo-ellipsoid. Here too dislocation activity is observed. In contrast to the triaxial case, initially only one side of the prismatic loop nucleates in a shear loop, due to the background shear stress. The flow resulting from these loops propagating out from the void acts to relieve the background shear stress so the triaxiality increases, as seen in Figure 3, and ultimately full prismatic loop activity is observed. It is interesting to note, however, that much of the void growth takes place under conditions of low triaxiality. Within the MD simulations the particular evolution of the stress triaxiality is strongly influenced by the initial purely uniaxial strain and the drop in the shear stress due to the ability of the void to emit sufficient dislocations, and to have them flow far enough, to significantly reduce the background shear stress in the box. The amount of shear stress reduction depends on the box size and hence the effective void nucleation site density. In any given system, experimental or computational, the nature of the plasticity is expected to depend on the extent to which plastic flow has increased the triaxiality at the point of void nucleation and growth. This flow of pre-existing dislocations not associated with void growth depends on the particular system and its history, but certain features are expected to be generic: Void growth can take place due to shear loop emission; Plastic flow increases the stress triaxiality; Under conditions of sufficiently high stress triaxiality the void growth Is due to prismatic dislocation loop emission.

[Fig. 3]

Coalescence of Two Voids

The linking of voids leading to the formation of the fracture surface is another important stage of ductile fracture. Often void nucleation is sufficiently sparse that the voids are initially well separated and grow independently for some period. As the voids grow larger, however, they enter a phase in which they interact with each other and multiple voids coalescence into a

single, larger void. We have studied this void coalescence process as two voids grow in a single crystal. We have observed that the voids do indeed follow the single void growth law initially, but as they grow sufficiently close to each other, they enter a phase of accelerated growth toward the neighboring void leading to coalescence. A question we wanted to address is whether there is a universal point at which this onset of coalescence begins. An old argument due to Brown and Embury [22] asserts that void coalescence begins when the voids are separated by one void diameter, and that the process is dominated by a shear mechanism as a slip plane connects the two voids. More recent continuum calculations by Horstemeyer and coworkers have predicted a larger coalescence distance of up to 7 void diameters. [23]

We have conducted atomistic simulations of void coalescence in a single crystal copper system oriented in the <100> directions in the simulation box and consisting of 120x120x120 unit cells and about 7 million atoms. [14,15] Two spherical nuclei were placed in the system, each with a radius of 1/20 of the box size. To avoid accidental bias due to the lattice symmetry, the nuclei were placed in a somewhat random (low symmetry) orientation with respect to each other. This orientation was kept fixed, while the initial separation distance of the voids varied from 1.0 to 1.8 void diameters over a series of simulations. During the simulation, the void surface was identified and tessellated, as described above, and the void separation (the inter-void ligament distance) was computed, as well as the diameter, volume, shape and other properties of the individual voids. The results are shown in Figure 4. The left panel shows atoms from a slice of the system including the centers of the two voids in which only atoms on the void surface, in dislocation cores or stacking faults are shown. Significant dislocation activity is evident around the voids as the material deformed plastically to accommodate the void growth. The right panel is a plot of the inter-void ligament distance normalized by the instantaneous value of the void diameter. Initially the inter-void ligament distance follows the smooth, solid curves. These curves indicate what the separation would be for two spherical voids of the same size located at the initial centers of the voids; i.e., what the separation would be if the voids did not interact. At a separation of roughly one void radius (indicated by the horizontal line in Figure 4), the voids begin to grow more rapidly toward each other as the coalescence process commences.

[Fig. 4]

On-the-fly Multiscale Modeling of Damage

The modeling of ductile fracture processes described thus far has used atomistic techniques. The advantage of an atomistic methodology is that the constitutive relations are packaged in the form of an interatomic force law that can be calculated from first principles. This force law together with the initial conditions determines the response of the material. The principal disadvantage of atomistic simulations, which must be weighed against the powerful atomic-level constitutive model, is that the length and time scales accessible to the simulation are quite limited. A cubic micron of material contains about 50 billion ($5x10^{10}$) atoms, which is just beyond the limit of the largest atomistic simulations to date. Atoms not only set the natural length scale, but the time scale as well. The Einstein frequency of atomic vibration sets a natural time scale characteristic of the

material, and the time step for explicit integration of the equations of motion must be short enough to integrate a period of motion accurately. For example in copper the Einstein frequency ω_E is roughly 30 THz, and we use a time step of 6.7 fs. The total simulation for multi-million atom systems is typically no more than a million time steps, so simulation time are limited to a few nanoseconds. Thus, large-scale MD simulations are limited to small volumes (<1 μm^3) and short times (<10 ns for multimillion atom simulations). For these reasons, more coarse-grained approaches to modeling the void processes are needed that can complement the atomistic modeling, and an extensive literature has been amassed on continuum modeling of ductile fracture.

We have developed techniques that are able to embed molecular dynamics in a continuum simulation, either using finite elements [24] or a more seamless technique known as coarse-grained molecular dynamics (CGMD) [25-27]. These techniques work best for inhomogeneous systems, in which there is only a relatively small region of the system where atomistic resolution is needed. The initial stages of void growth comprise such a system, since the plasticity occurs near the void surface, and yet the long-range strain fields that emanates from the void requires a large peripheral volume to be simulated. Rather than using atomistics in the periphery, a computationally much less expensive finite element model can be used to model the elastic fields, coupled to atomistics that capture the dislocation nucleation and initial propagation near the void. We have conducted this kind of concurrent multiscale modeling of voids, but we do not have the space to report the results here.

Another multiscale approach we have taken involves calculating constitutive information for a finite element simulation on the fly from a fine-scale model that describes physics at shorter length scales than are supported on the mesh. In one case we have modeled damage localization using a DFRACT model to describe the void nucleation, growth and linking at the fine scale. In principle the fine-scale model would apply in each representative volume (material point) of the coarse-scale simulation, but a computational advantage can be gained by using a coupling layer to initiate a fine-scale calculation only when it would provide new information. In some cases, the conditions at the coarse scale are such that it is known that little or no void growth would occur; in other cases, a fine-scale calculation with essentially the same state and conditions will have already been performed, and a call to the database can provide the answer without a new fine-scale calculation. The results from a one-dimensional damage calculation are shown in Figure 5 for two sets of parameters. [28] In one case (Figure 5 left panel) the material parameters favored localization due to heating, and the sampling approach was very effective with only 1 out of every 203 calls for constitutive data requiring a full fine-scale model calculation. In the other case (Figure 5 right panel), there was less localization and 1 out of every 26 calls resulted in a fine-scale model calculation. If the fine-scale calculation is very expensive computationally (e.g., a molecular dynamics simulation), this low sampling rate gives a dramatic speed up to the simulation. In another application, a sophisticated database management and extrapolation technique was developed based on a generalization of the in situ adaptive tabulation technique used in combustion simulations. [29] The technique was

applied to model large plastic deformations in shock waves and in systems with shear localization based on a crystal plasticity model. [30]

[Fig. 5]

Conclusions

We have used large-scale atomistic simulations and multiscale methodologies to investigate the void processes involved in ductile fracture. New analysis techniques have been developed in order to extract physically relevant quantifications of the void behavior that can be compared with experiment and continuum modeling. In the case of the study of void growth under low triaxiality, we found a prolate-to-oblate transition that has been understood in terms of the elastic and plastic phases of the deformation. In the case of the void coalescence study we have identified a critical inter-void ligament distance at which the onset of void coalescence occurs.

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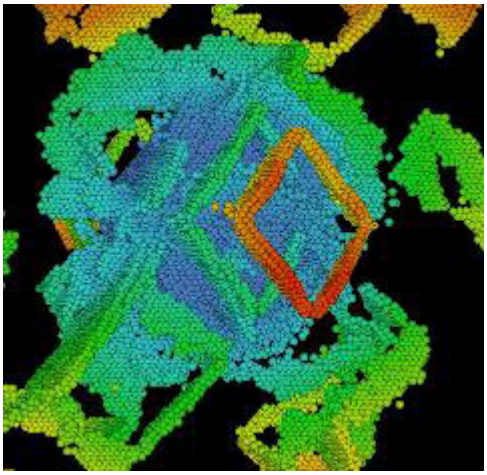

Figure 1. Dislocations emitted during the growth of a single isolated void in copper. Each sphere represents an atom, colored according to the distance from the center of the void. Dislocation loops are formed in response to the resolved shear stress at the void surface, and act to transport material away from the void as it grows [2]. Only atoms in dislocation cores, stacking faults or on the void surface are shown.

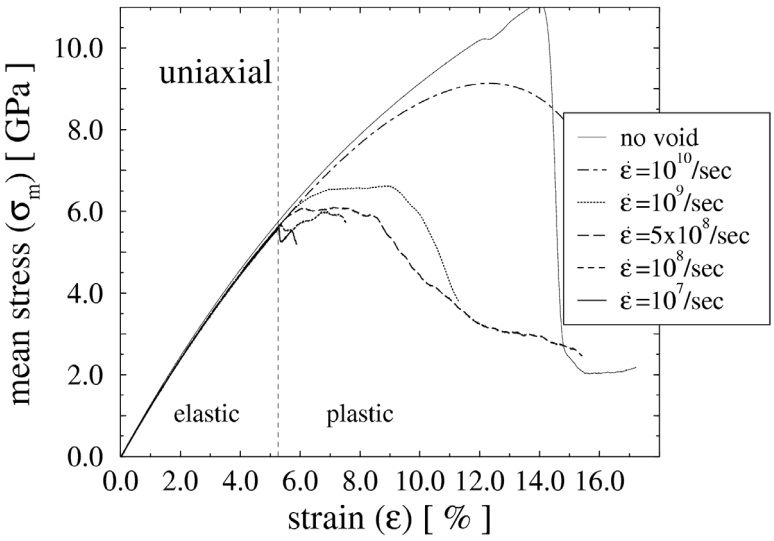

Figure 2. Stress-strain curves for void growth in copper during uniaxial expansion at the strain rates shown. In the cases other than "no void" the growth began with a spherical nucleus. The initial elastic phase (indicated roughly by the vertical dashed line) is followed by a plastic phase in which the mean stress is reduced compared to the elastic mean stress represented by the "no void" curve. Eventually, even the no void system is unstable to cavitation and the stress drops. Significant rate dependence is observed once plasticity begins. [13]

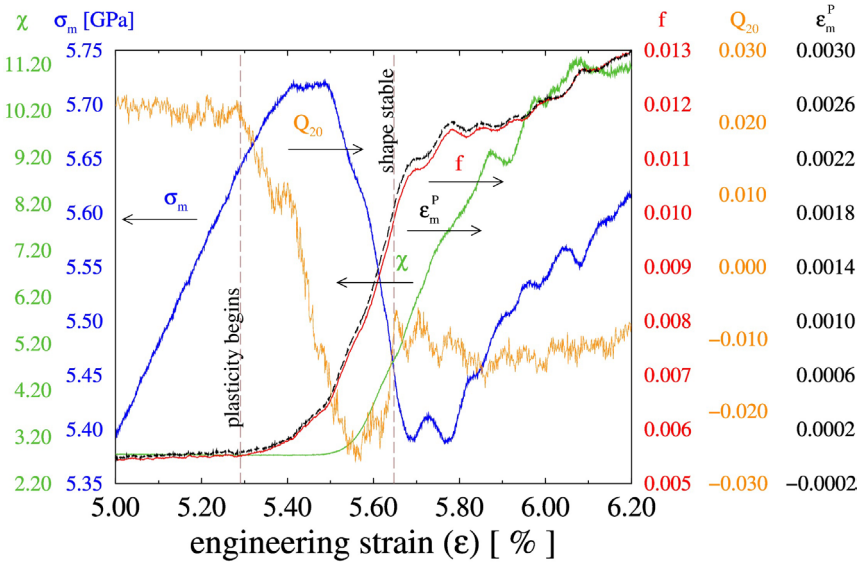

Figure 3. Quantities characterizing the void growth process during uniaxial expansion of copper at a strain rate of 10^8/s. The mean stress σ_m rises initially due to the expansion and then drops due to the void growth. The void volume fraction f and the mean plastic strain ε_m^p quantify the size of the void, and show remarkable agreement. The quadrupole moment Q_{20} quantifies the eccentricity of the void, and transitions from a positive (prolate) value to a negative (oblate) value. The stress triaxiality χ increases as the shear stress is reduced due to plastic flow. The vertical lines indicate when dislocations form ("plasticity begins") and when the dislocation activity has led to a roughly constant value of Q_{20} ("shape stable"). [13]

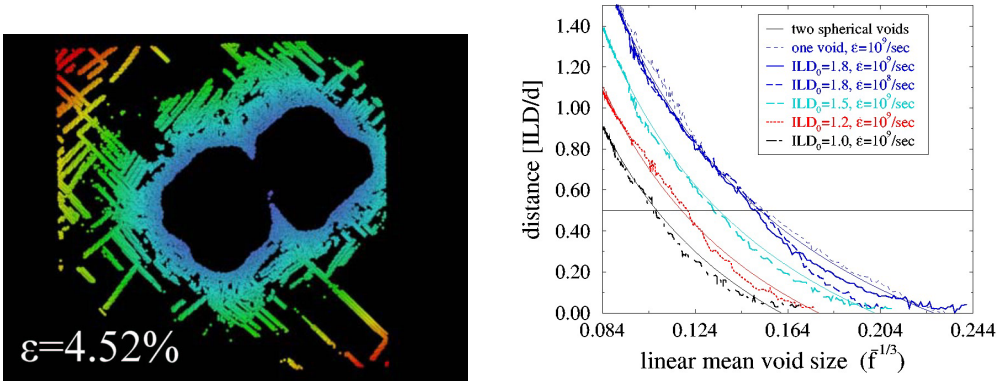

Figure 4. Coalescence of two voids in copper, as shown in the left panel at a strain of 4.52% just after the voids coalesce. The right panel is a plot of the inter-void ligament distance (ILD) normalized by the instantaneous void diameter vs. the linear void size (the cube-root of the single void volume fraction). The different data sets correspond to different initial separations of the voids: ILD_0 = 1.0, 1.2, 1.5 and 1.8 times the initial void diameter. The horizontal line indicates the point at which the voids begin to interact. [14]

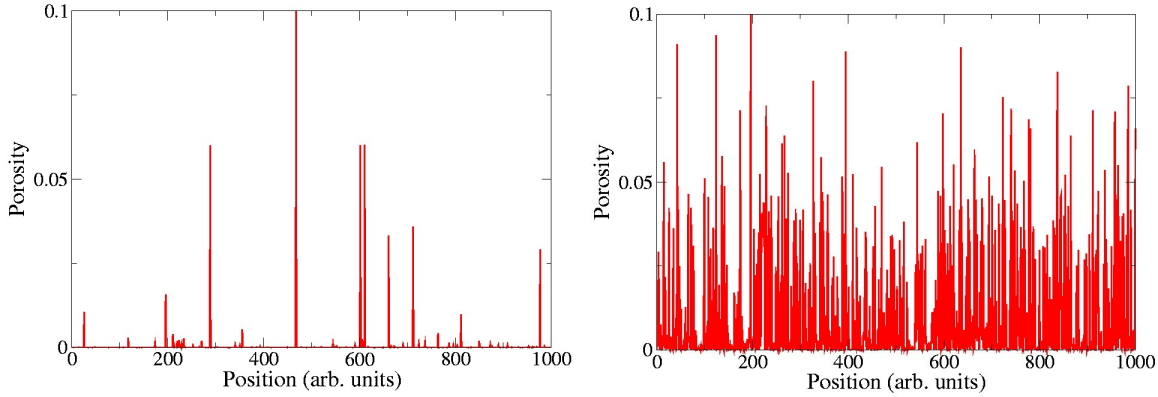

Figure 5. Damage localization simulations with plots from runs with two different sets of material parameters. [26] Each plot shows the porosity in each element of the one-dimensional simulation. In the more localized case (left), an actual fine-scale model calculation was needed less than 1% of the time; in the other case (right), it was needed 4% of the time. With expensive fine-scale models, this low sampling rate can greatly speed up the simulation.