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Surface effects at the nanoscale significantly reduce the effects of stress concentrators

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Abstract

At nanoscales, the large surface over volume ratio is shown to be instrumental in eliminating or significantly reducing the adverse effects of nanoscale stress concentrators (NSCs) such as impurities, inclusions, pores, and cracks. Using molecular dynamics (MD) simulations, Cu crystals with and without NSCs are strained in tension and in shear, at two strain rates, one being an order of magnitude larger than the other. Cube-shape crystals with periodic boundary conditions show sensitivity to NSCs similar to macrosize samples where fracture mechanics works well. For such crystals, atomistic defects cluster near the loaded surfaces, the clustering being stimulated significantly by the NSCs. Crystals with non-periodic boundary conditions, however, show insensitivity to NSCs, for the sample sizes examined herein, i.e., cubes up to about 30 nm side length. Atomistic defects do not cluster near the loading surfaces but rather distribute over the entire sample. Even though the spatial distribution of atomistic defects depends on the presence of NSCs, the total number of such defects is found to be independent of the presence of NSCs for the cubic crystals. The reason for this is the presence of a "vast" amount of surfaces, for the non-periodic boundary conditions case, where numerous atomistic defects initiate, making the number of defects initiating from NSCs insignificant. Provided that the average energy in creating these defects is constant, a robust explanation of the insignificance of NSCs emerges.

Keywords: Stress concentrators; Nanoscale; Surface effects; Material reliability

1. Introduction

Materials show size effects, for example, improved properties such as strength as size decreases. The study of size effects traces back to the works of Leonardo da Vinci and Galileo Galilei, mostly addressing macroscales; [1] cites 377 works on the subject mostly at scales from centimeters to several meters. A "simple" reasoning is that larger-sized samples show a reduction in strength for probabilistic reasons: a larger sample simply has more flaws to initiate cracks. At the same time, surfaces interact strongly with the material microstructure (including defects) and thus contribute significantly to size effects [2,3]; note that in a general sense surfaces are discontinuities or flaws. As the size decreases, the ratio of surface over volume increases, to the point that for size small enough, it is surfaces that dominate the initiation of atomistic defects, making the presence of NSCs insignificant. The question how small is small enough for this to occur is not easily answered. Evidence shows that "small enough" implies the nanometer range, where atomistic behavior is dominating. In [4] very encouraging preliminary results on the subject were presented on this topic. These results are in line with the reasoning presented in [5] where, based on linear elastic fracture mechanics and numerical simulations, clear evidence is presented that as the size approaches atomic dimensions, the theoretical material strength should be approached.

Nanoscale stress concentrators (NSCs) here indicate defects such as impurities, inclusions, cracks, pores; defects other than NSCs, for example dislocations, are also addressed, yet they are considered part of the "bulk" material, thus they are not considered, terminology wise, as NSCs. NSC defects are present even in nanostructural materials; for example, a membrane of thickness in the nanometer range will contain NSCs from the roughness of the substrate on which it was deposited, from impurities, pores, inclusions, etc. There is a wealth of information on material properties at nanosizes, yet

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most address "ideal" conditions, i.e., do not include the effects of NSCs, even though they are rather ubiquitous. Additionally, a robust design must consider the possibility of NSCs in nanostructural materials.

The objective of this paper is to provide detailed evidences for significant surface effects in materials of nanodimensions.

2. Simulations

Simulations of single FCC Cu(001) crystals with and without NSC defects are reported, where the embedded atom method (EAM) for molecular dynamics (MD) simulations was employed; the applicability of the EAM for the study of the deformational behavior of metals such as the ones in this work is well documented in the literature. More involved methods based on tight-binding and ab initio calculations not only limit the size of the systems to be solved but impose an unneeded complication to the problems herein. The EAM [6–8] is a semi-empirical many-body potential, based on density functional theory. The EAM suggests, in part, that the energy required to place an impurity atom in a lattice is determined by the electron density at that site, irrespective of the source of the electron density.

EAM simulations within the parallel MD program ParaDyn [9] modified for the purposes herein were performed on an HP supercomputer, using 64 EV-7 processors. Two sizes of three-dimensional cube-shaped crystals were simulated. For the first one, the edge length along the three axes, x, y, z, was equal to 28.88 nm (2,048,000 atoms, thereafter termed as the "large"); for the second one the edge length was 18.05 nm (500,000 atoms, thereafter termed as the "small"). In addition to straining the initially perfect crystals, the small and large crystals containing an NSC of $3.0 \times 3.0 \times 0.4$ nm^3 (shorter dimension in the z-direction, here termed as NSC-1) positioned at their center were strained as well. In addition, large size crystals containing a larger NSC of $3.5 \times 3.5 \times 1.6$ nm^3 (shorter dimension in the z-direction, here termed as NSC-2), were strained. These NSCs are voids/pores, yet their 90° corners (270° material corners at the pore, with pairs close to each other) imply a singularity similar to a crack within a mechanics of materials framework.

Three types of straining were imposed.

(i) The crystals were strained in the z-direction (tensile straining) at constant strain rate by fixing the atoms in the lower z-border-plane and by imposing constant velocity on the atoms in the upper z-border-plane. Constant velocity was imposed by assigning an initial velocity in the z-direction to the atoms in the upper z-border, and then setting the force on these atoms throughout the simulation, in all three directions, equal to zero.

(ii) Here the atoms in the lower z-border-plane are fixed, while the atoms in the upper z-border are assigned a constant velocity in the y-direction. Similarly to straining (i), the force on these atoms, in all three directions, was set equal to zero. This is a so-called "simple shear" straining within a mechanics of materials terminology (as opposed to pure shear). Here, stress concentrations at the corners are not as intense as in case (i).

(iii) The atoms in the lower z-border-plane were forced to move on their initial z-plane only, and constant velocity is imposed to the atoms at the upper z-border. Constant velocity was imposed by assigning an initial velocity in the z-direction to the atoms on the upper z-border, and then setting the force on these atoms throughout the simulation, only in the z-direction, equal to zero. This differs from straining (i) since the atoms on both z-borders are allowed to move on the z-plane, thus avoiding stress concentrations at the corners due to Poisson effects.

The imposed velocity for all three straining cases was such that the strain rate was either 10^8/s, herein termed as the "slow" strain rate, or 10^9/s, termed as the "fast" strain rate. Two types of boundary conditions on the x- and y-planes were used, one non-periodic and one periodic. The latter represents an infinitely large sample in x and y, within the restrictions of the periodic boundary conditions, thus it does not represent a true infinite problem in the x- and y-directions but rather a periodically infinite problem. In all simulations, the initial temperature was 300 K, and it was maintained at that temperature throughout the simulation by a Hoover drag (damped) thermostat (built-in in the ParaDyn routine).

Fig. 1 shows the stress–strain response of the large and small crystals with and without NSCs subjected to slow strain rate, straining case (i). The stress–strain response is insensitive to the presence of the NSCs. However, as shown in Fig. 2, this is not the case for the periodic boundary conditions. Note that the periodic case implies infinite dimensions in the x- and y-directions, yet not an infinite crystal in these directions, but rather a periodic one. As detailed further in the sequence, these boundary conditions are not the same as the non-periodic ones when it comes to initiating defects, which, according to the thoughts advanced in this work, account significantly for the material behavior at such small scales.

Based on these results, the existence of a scale h_{cr} below which this insensitivity appears is conjectured [4]. In more detail, Fig. 3 shows a schematic on this, i.e., the h_{cr} depends on the relative value of the sample size to the NSC size. For a given value of the NSC diameter, say 50% of the thickness allowance for design purposes, a definite value of h_{cr} is defined, where the surface in Fig. 3 reaches a constant strength value. Identification of h_{cr} for several materials would provide a new opportunity for creating structurally efficient materials based on nanosize components.

The stress–strain plots presented above do not, alone, provide an understanding of the effects of the NSCs. The initiation, propagation, and distribution of atomistic defects during loading should be investigated for this purpose. An atomistic defect is defined to occur at those spatial positions where an atom's coordination number changes from that of the intact crystal (for FCC, the coordination number for a bulk, i.e., not on the surface, atom is 12); atomistic defects forming a line in space indicate a dislocation, while other defects can be identified similarly. In the following, N indicates the total number of atomistic defects, which may or may not be related to the total number of dislocations. If atomistic defects are mostly in the form of dislocations, then, provided the mean dislocation

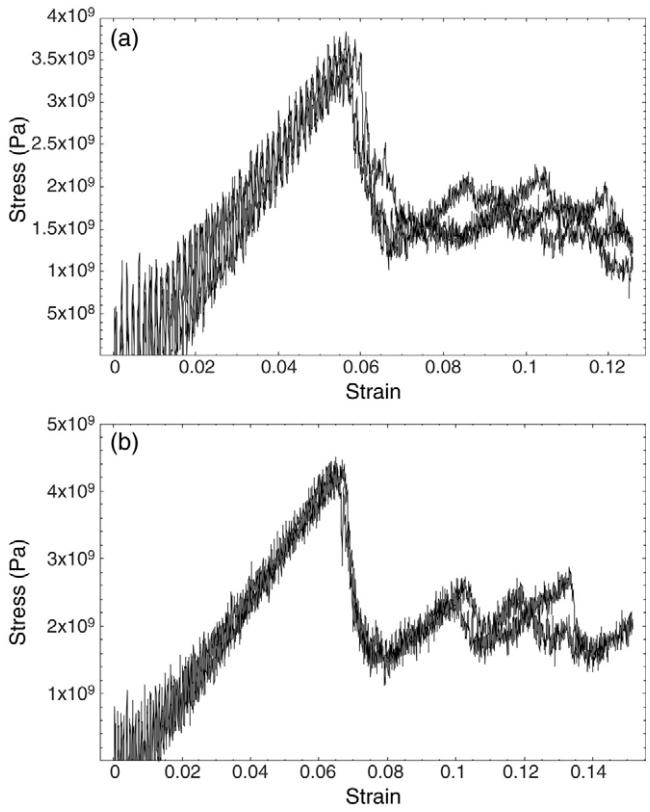

Fig. 1. Stress versus strain response for non-periodic boundary conditions and slow strain rate under straining case (i). (a) Three curves for the large crystal, i.e., for the intact one, and for the ones with NSC-1 and NSC-2. (b) Curves for the small crystal, for the intact and for the one containing the NSC described in the text.

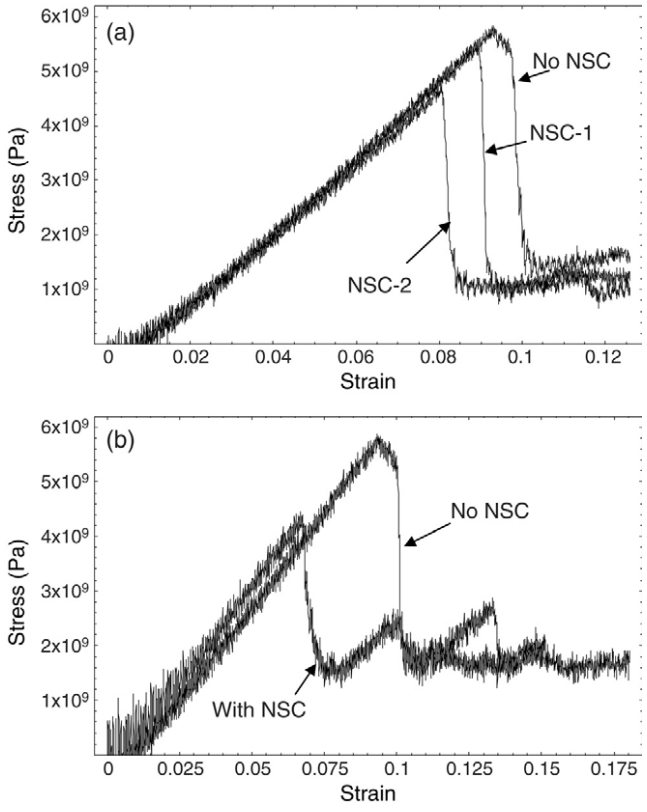

Fig. 2. Stress versus strain response for periodic boundary conditions and slow strain rate under straining case (i). (a) Three curves for the large crystal, i.e., for the intact one, and for the ones with NSC-1 and NSC-2. (b) Curves for the small crystal, for the intact and for the one containing the NSC described in the text.

length is constant, N also indicates a number proportional to the number of dislocations. N is used to characterize the structural evolution of defects in the crystal. Fig. 4 shows the number of atomistic defects N that develop during straining plotted at five strain levels, for the non-periodic boundary conditions and the slow strain rate case. Even though the pattern of deformation-induced defects is spatially different in the crystals with the NSC than those without it, the load versus displacement or average stress (total force per area) versus strain (average displacement over initial length) curves are independent of the presence of the NSC for the cases examined, as shown in Fig. 4. If on average the energy required in creating such defects is constant, this explains the insensitivity to NSCs. However, the spatial distribution of such atomistic defects should not be clustered for this argument to be valid. Such clustering occurs in the samples with periodic boundary conditions, as will be discussed in the following. Before addressing this important point, note that, as shown in Fig. 5, N depends strongly on the presence of NSCs for the periodic boundary conditions case.

Fig. 6 shows the atomistic defects in three-dimensional view for the five strain levels at which Fig. 4(a) was plotted. Up to about the peak strength, deformation-induced atomistic defects are distributed more or less homogeneously over the entire sample, with little, if any, concentration in the area of the NSC. Yet, in the vicinity of the peak strength, long-range atomistic defects, mainly in the form of dislocations and stacking faults,

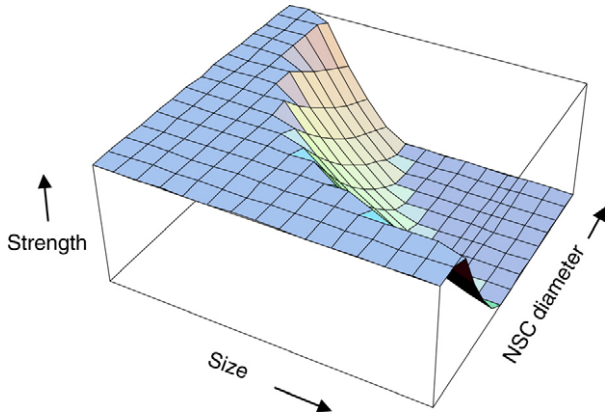

Fig. 3. Schematic on the definition of the critical sample size, e.g. thickness (size) of a ply/film loaded in the direction transverse to its thickness, h_{cr}, as a function of the NSC size.

form. As expected, the crystal without any NSC forms isolated slip planes (111) while the one with the NSC forms several slip planes. Even though the NSC is a defect initiation source, the vast amount of surfaces in such small volumes – for a cube, the surface area over volume is $\sim 1/a$, a denoting the side of the cube – seem to initiate the majority of defects (including numerous dislocations) which finally lead to several slip planes, interrupted in the bulk of the crystal by the NSC. Similar observations hold for the small crystal with and without

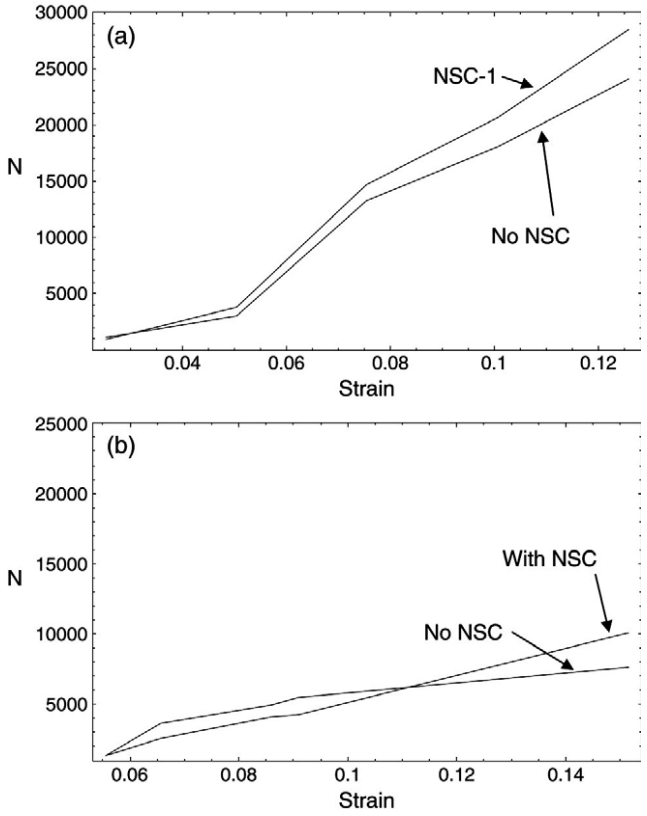

Fig. 4. Number of atomistic defects N as a function of strain, at five strain levels during deformation at the slow strain rate, for non-periodic boundary conditions and straining case (i). (a) For the large sample with initial NSC-1 and without NSC; (b) for the small sample with and without initial NSC.

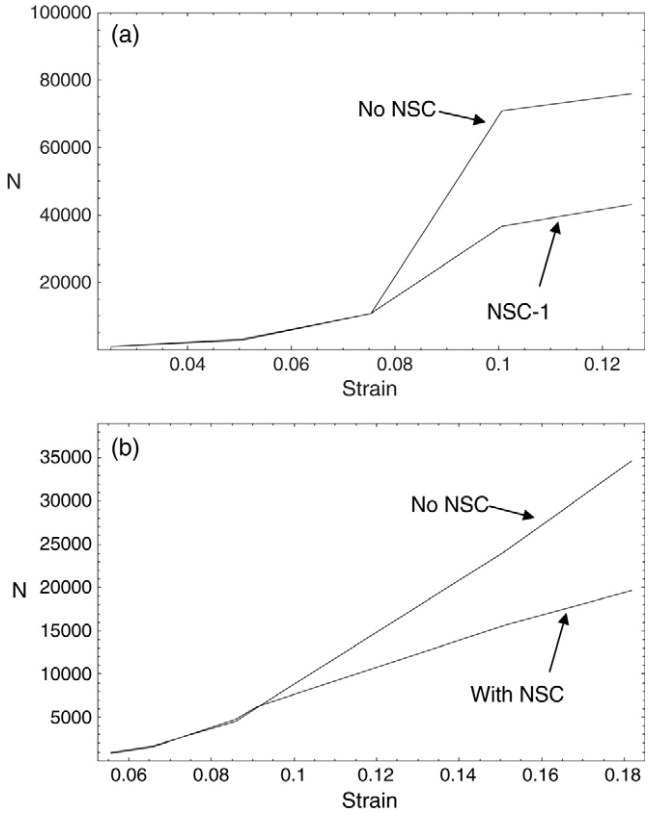

Fig. 5. Number of atomistic defects N as a function of strain, at five strain levels during deformation at the slow strain rate, for periodic boundary conditions and straining case (i). (a) For the large sample with initial NSC-1 and without NSC; (b) for the small sample with and without initial NSC.

the NSC; for compactness, the relevant graphs are not shown herein.

It is noted that the triangular slip planes in Fig. 6 are expected for the given straining and crystal orientation [10]. This suggests that the stress concentrations at the corners are weak, thus the differences in material behavior between straining cases (i) and (iii) should also be small. This interesting point is examined in more detail in the sequence.

Fig. 7 shows the atomistic defects in three-dimensional view at five strain levels (the same strain levels at which Fig. 5(a) was plotted), while Fig. 8 shows the side view of the atomistic defects. Again, up to about the peak strength, deformation-induced atomistic defects are distributed nearly homogeneously over the entire sample, with little, if any, concentration in the area of the NSC. As opposed to the non-periodic boundary conditions case, atomistic defects tend to cluster near the loading surfaces (top and bottom) especially in the vicinity of the peak strength. The total number of defects N grows faster, at increased strain levels, for the sample containing the NSC than the one without the NSC. Given that the presence of the NSC reduces the peak strength, one concludes that the clustering of defects is paramount in this case. Defects initiate from the free surfaces and the NSC and quickly become trapped at the loading surfaces. Thus, it is the clustering of defects, rather than the total number N, that dominates peak strength and inelastic deformation in the case of the large (infinite) lateral dimensions modeled by periodic boundary conditions.

For the fast strain rate case, the results are similar to the ones presented above, showing that the strain rate does not alter the central theme of this paper. Fig. 9 shows the spatial pattern of atomistic defects that develop during the high rate straining of the large sample containing NSC-1. The rapid proliferation of defects near the peak stress is noted.

Based on linear elastic fracture mechanics, the stress intensity factor for the crystal containing an NSC under non-periodic boundary conditions is approximately the same as that for the same crystal containing the same NSC under periodic boundary conditions, e.g. [11] (considering plane strain or plane stress conditions and isotropic constitutive response). Then, differences in behavior between the periodic and non-periodic boundary conditions cannot be attributed to differences in stress intensity, which strengthens the theme and claims of this paper on the importance of surfaces.

2.1. Stress concentration at the corners

Straining case (i) does not allow the atoms on the upper and lower z-border-planes to move in the x- and y-directions. This creates a stress concentration at the corners due to Poisson effects. Comparing results from straining cases (i) and (iii) should indicate how contributing this stress concentration at the corners is, compared to that from the NSCs. Additionally,

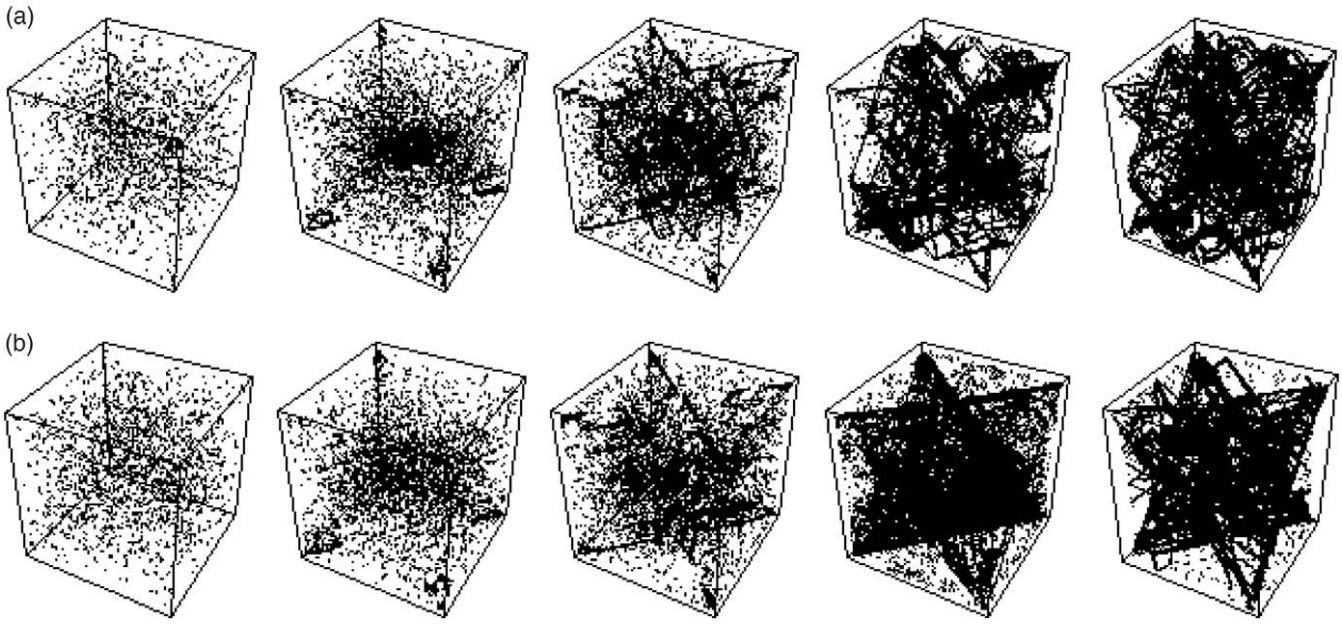

Fig. 6. Three-dimensional plot to atomistic defects for the five strain levels at which Fig. 4(a) was plotted. (a) Large sample with initial NSC-1. (b) Large sample without any initial NSC. Both plots are for non-periodic boundary conditions and the slow strain rate.

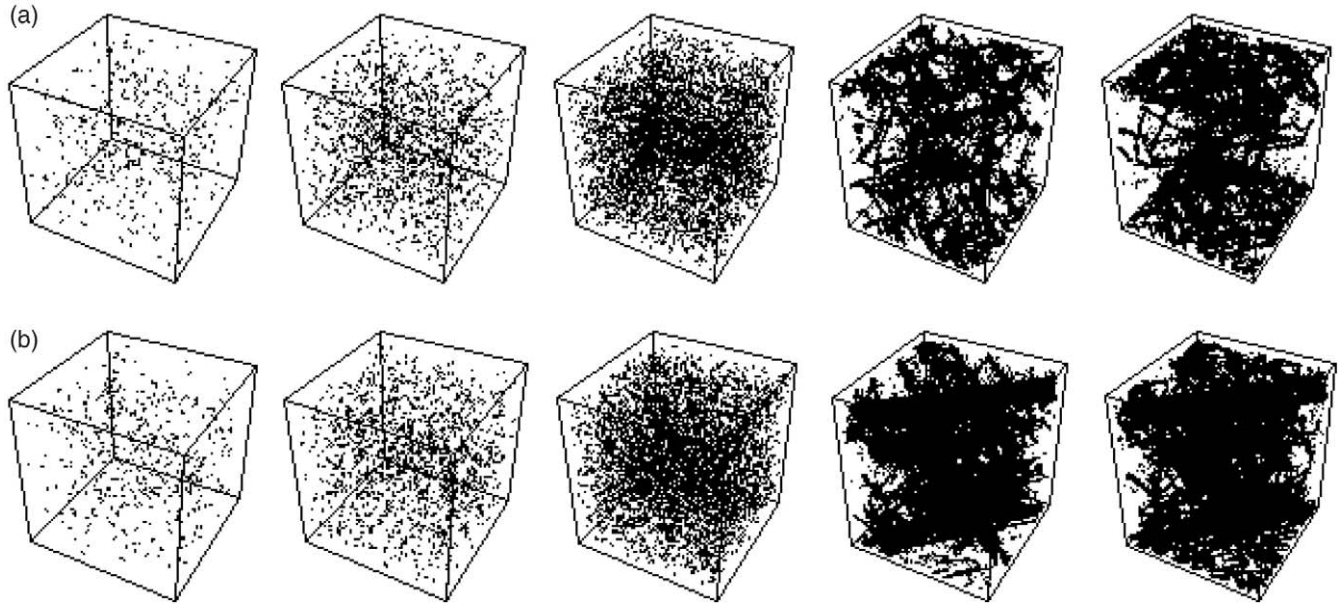

Fig. 7. Three-dimensional plot of atomistic defects for the five strain levels at which Fig. 5(a) was plotted. (a) Large sample with initial NSC-1. (b) Large sample without any initial NSC. Both plots are for periodic boundary conditions and the slow strain rate.

straining case (ii) should also provide information on this issue, since the stress concentrations at the corners are not as pronounced as in straining case (i).

Figs. 6 through 9 show some concentration of atomistic defects at the corners, yet those seem to be of limited extent and rather concentrated in a small volume in the vicinity of the corners. Some results from straining cases (ii) and (iii) are presented herein, not as extensively as for case (i), for the sake of compactness. For straining case (ii), Figs. 10 and 11, show that the effects of the NSCs are similar to those for case (i). However, the small reduction of peak stress value for the non-periodic crystals with NSCs indicates some influence of the stress concentrations at the corners, but not a significant one. Similar considerations hold for straining case (iii), as shown through Figs. 12 and 13. Comparison of Fig. 13 with Fig. 1(b) shows a small, yet not as significant effect of the stress concentration at the corners for straining case (i). The same conclusion can be made by comparing Fig. 12(a) with Fig. 12(b). Finally, it is mentioned that for both loading cases (ii) and (iii) the evolution of the number of atomistic defects follows trends very similar to those for case (i).

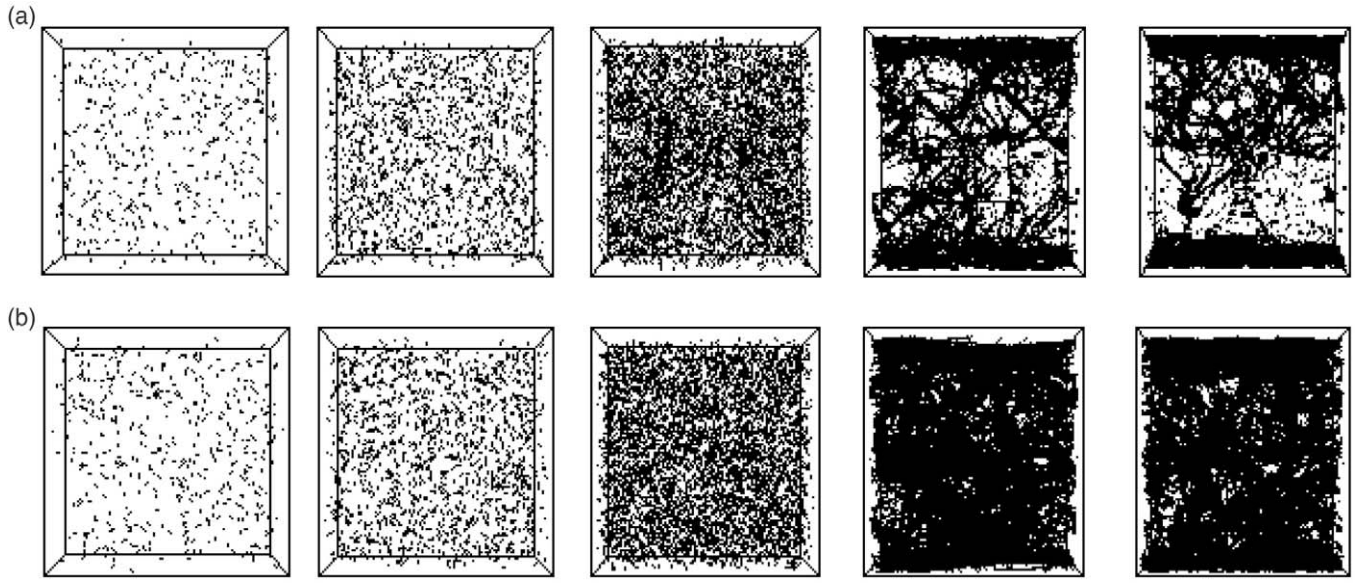

Fig. 8. Side views of the plot shown in Fig. 7. (a) Large sample with initial NSC-1. (b) Large sample without any initial NSC. Both plots are for periodic boundary conditions and the slow strain rate.

Table 1
Reduction in peak stress for the small crystal with the NSC as compared to the intact crystal, for slow strain rate

	Reduction in strength for non-periodic boundary conditions (%)	Reduction in strength for periodic boundary conditions (%)
Straining case (i): strong Poisson effects for non-periodic problems	0	34
Straining case (ii): moderate or minimal Poisson effects for non-periodic problems	8	41
Straining case (iii): no Poisson effects	9	34

The strength drops were measured from the relevant figures using the process described in the text.

Table 1 shows the reduction in peak stress for the small crystal with the NSC as compared to the intact crystal, for all three straining cases (i)–(iii) and the slow strain rate. Even though the vibrational noise depicted in the stress strain curves as fluctuations is often high, thus hindering a robust direct measurement of the peak stress, for the slow strain rate and the small crystals, the practically vertical drop in stress after the peak provides an indication of the reduction in strength. Thus, the percentage reduction in strain at the peak stress provides an estimate of the percentage reduction in peak stress. These fluctuations also point to the need for a probabilistic approach to the problem, as explained in further detail in the following section. The values indicate clearly that the Poisson effects and the relevant stress concentrations at the corners is not the prime reason for significantly reducing the effects of the stress concentrators. It is the surfaces that are primarily responsible for this significant reduction.

3. Probabilistic, experimental issues and future outlook

Simulations along the lines of this paper allow one to perform “experiments” that are very difficult, often impossible, for the laboratory. Even though the atomistic material behavior at such scales is inherently probabilistic, from the initial velocities and position of the atoms, the tendency of atoms near surfaces to be “uncomfortable” there or even unstable, etc., due to computer power limitations usually single realizations are studied. As the size of the samples increases, for example in the multimillion atom range, single realizations may provide adequate information. A non-systematic study has revealed that curves such as those in Figs. 1 and 2 do not change for realizations with different initial velocities of the atoms. Even though the probabilistic aspects of this work provide one link to the “probabilities and materials—from nano to macro workshop” where it was presented, there is a potentially stronger link. It pertains to the effects of stress concentrators, where the work reported herein may shift the way strength and (probabilistic) reliability of relevant materials, for example laminates with plies of thickness in the nanometer range, are studied.

Even though experimental results complementary to the simulations are not addressed herein, some experimental issues are discussed, as well as some simulation issues of larger scale samples and structures with nanodimensions. Laboratory capabilities are limited, and one common test for examining mechanical behavior at nanoscales is nanoindentation, the small-scale version of the traditional hardness test, used especially for elucidating the mechanical properties of thin films. An extensive number of simulation and experimental studies are available in the literature, for example [12–20],

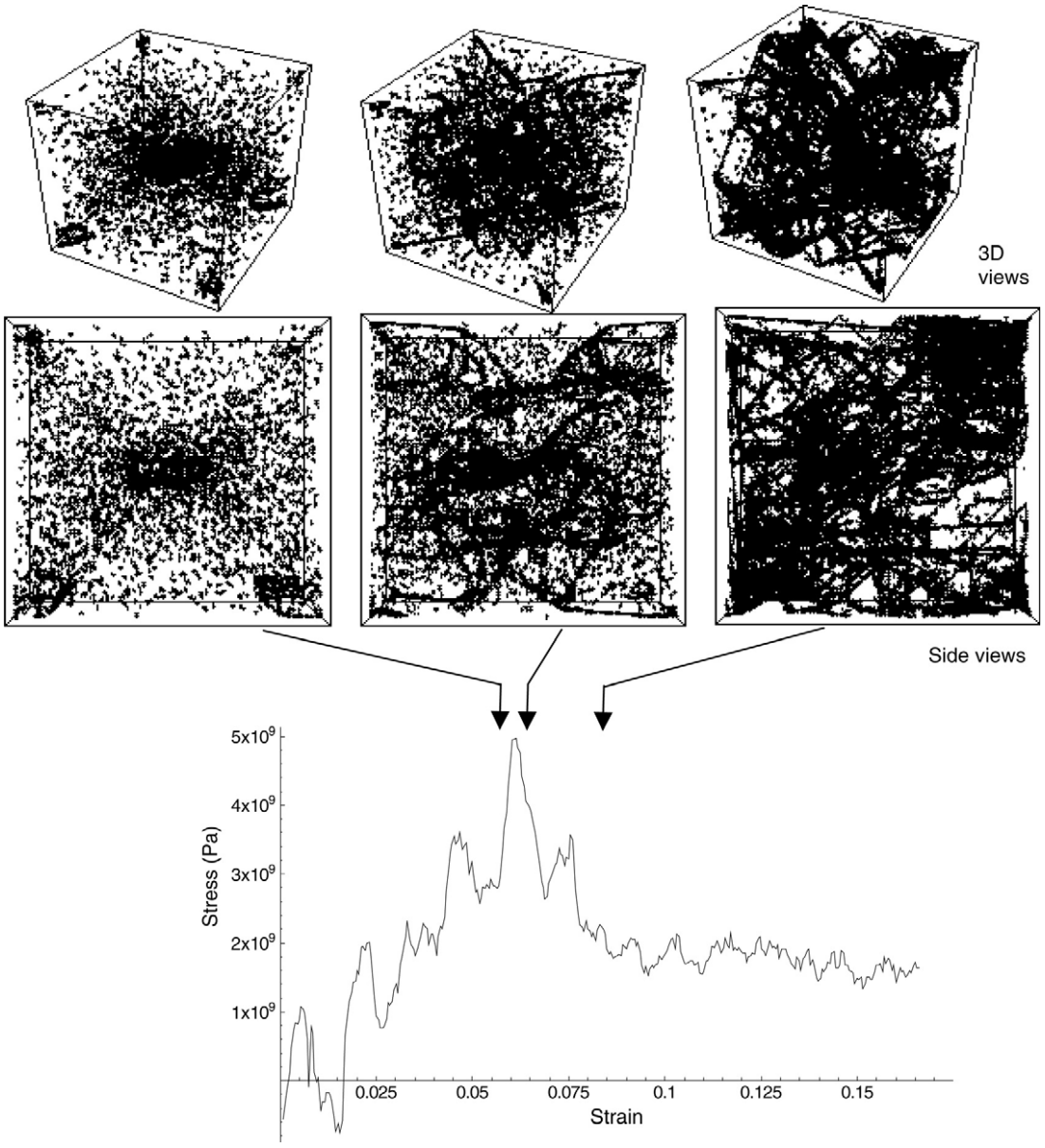

Fig. 9. Atomistic defects and stress–strain plot for the large sample containing NSC-1 and loaded at the high strain rate under non-periodic boundary conditions and straining case (i). Top row: 3D views at strain levels 0.055, 0.065, and 0.085, respectively. Bottom row: side views at strain levels 0.055, 0.065, and 0.085, respectively.

with interesting results such as effects dependent on the radius of the indenter, phase transformations during indentation, effects of the substrate properties, and thickness of the film. The work reported herein seeks the effects of NSCs and the dependence of these effects on their size and the structural size, information that is difficult to deduce from nanoindentation. The very local indenter, which introduces an NSC, interacts strongly with pre-existing NSCs; two samples (films of different thickness) are unlikely to have the same NSCs positioned near the indenter in a similar fashion. This introduces, naturally, probabilistic aspects in the problem. Similar probabilistic issues are applicable to the results presented herein, not only with respect to the position and size of NSCs. Important ones include temperature and vibrational properties of the atoms, sensitivity to boundary conditions (especially given the unstable position of atoms near boundaries such as free surfaces), the statistical distribution of defects during deformation and whether stationarity of any kind can be claimed. Even though these were not examined in the present study, it is our belief that due to their importance they will receive increasing attention, especially in the research community that publishes in this journal.

Various other methods, besides nanoindentation, exist for mechanical testing in small dimensions, mostly for films. Microtensile testing [21], bulge testing [22], and microbeam deflection [23,24] are some, while MEMS (Micro Electromechanical Systems) tests are emerging as an alternative [25,26]. For the issues addressed in this work, some of these methods may be useful. We are presently designing experiments that can also be simulated, i.e., experiments

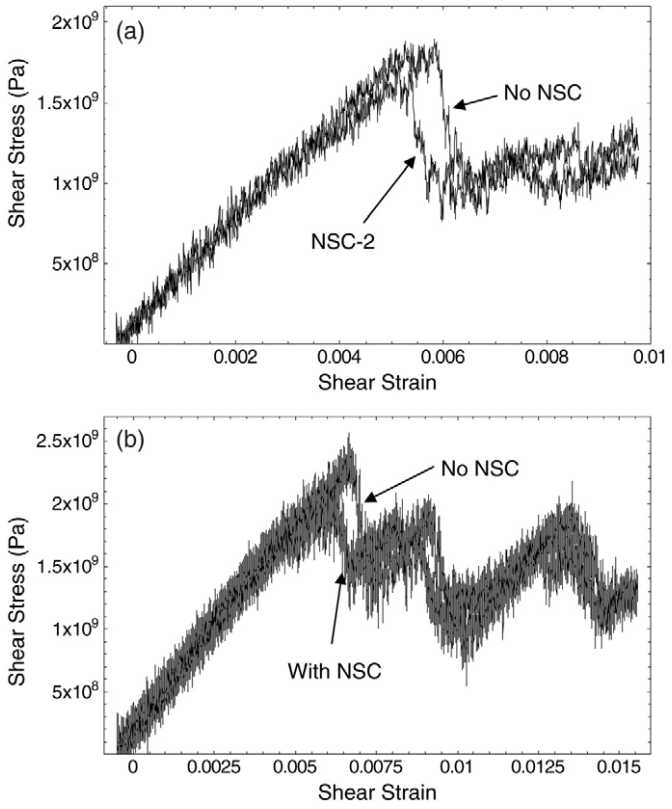

Fig. 10. Shear stress versus shear strain response for non-periodic boundary conditions and slow strain rate, straining case (ii). (a) Two curves for the large crystal, i.e., for the intact one, and for the one with NSC-2. (b) Curves for the small crystal, for the intact one and for the one containing the NSC described in the text.

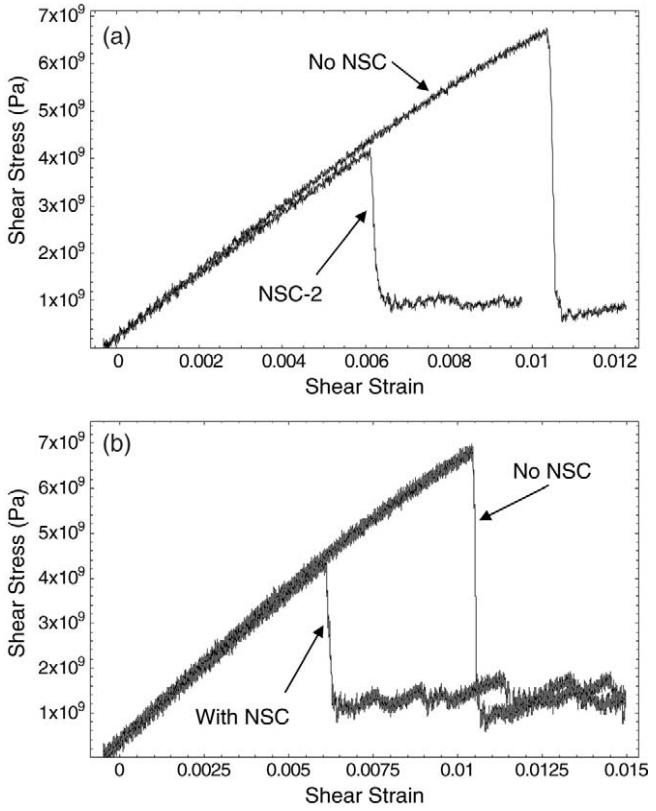

Fig. 11. Shear stress versus shear strain response for non-periodic boundary conditions and slow strain rate, straining case (ii). (a) Two curves for the large crystal, i.e., for the intact one, and for the one with NSC-2. (b) Curves for the small crystal, for the intact one and for the one containing the NSC described in the text.

for which: (a) the sample has easily identifiable hot spots which contain defects identifiable by the experiments and their behavior can be simulated; (b) residual stresses in the material are eliminated or reduced, which after all are very difficult and often expensive to measure [27]; (c) using relatively smooth probes for loading of membranes and tubes, sharp externally imposed localized deformation is avoided; (d) the probabilistic nature of the problem is taken into account in designing the experiments and analyzing the results.

For simulating larger-scale problems, and slower strain rates, multiscale simulations are necessary. A large part of multiscale work is devoted to modern simulation methods involving coupling of length scales and sometimes time scales. Simulation methods for coupling length scales can be characterized as either serial or concurrent. In serial methods a set of calculations at a fundamental level (small length scale) is used to evaluate parameters for use in a phenomenological model at a longer length scale. For example, atomistic simulations can be used to deduce the constitutive behavior of finite elements (FEs), which can simulate larger problems. Limitations of these methods include that small scale phenomena are parameterized in these studies through defect geometries that fit within the size of the FEs and may thus not capture the full complexity of a hypothetical fully atomistic system. A way to address this limitation is to use concurrent methods, which rely on coupling seamlessly different computational methodologies applied to different regions. For example, atomic simulation techniques are used to model the crack tip where large deformations (even bond breakage) occur and continuum approaches (FE methods—which can also have information passed from smaller scales) are used to model the region far away from the crack tip. For problems of extensive inelastic deformation, for example long dislocations or microcracks traveling from the atomistic to the continuum region, such methods become difficult to deal with; some recent attempts [28], however, are encouraging in addressing the difficulties.

The quasicontinuum (QC) method has emerged as a powerful multiscale simulation method [29]; comprehensive reviews can be found in many recent publications, such as [30, 31]. Its extension to finite temperatures is addressed in [32]. In the QC method, two types of atom are identified, i.e., local representative atoms and non-local representative atoms, instead of identifying atomistic and continuum regions. Even though the method appears as a serial multiscale method, in practice, the regions containing non-local representative atoms are essentially equivalent to the fully atomistic regions of the concurrent multiscale methods; however, a major advantage of the QC method is that these regions adapt according to the deformation field.

In multiscale methods, a major concern is that the evolution of the system is controlled by the atomistic simulations,

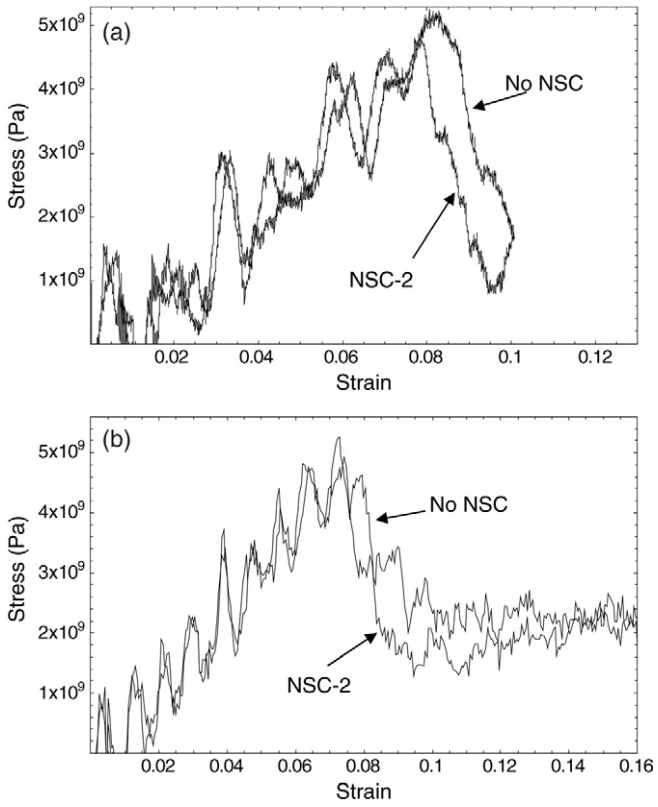

Fig. 12. Stress versus strain response for non-periodic boundary conditions and fast strain rate, straining case (iii). (a) Two curves for the large crystal, i.e., for the intact one, and for the one with NSC-2. (b) Curves for the same crystals as in (a), yet for straining case (i).

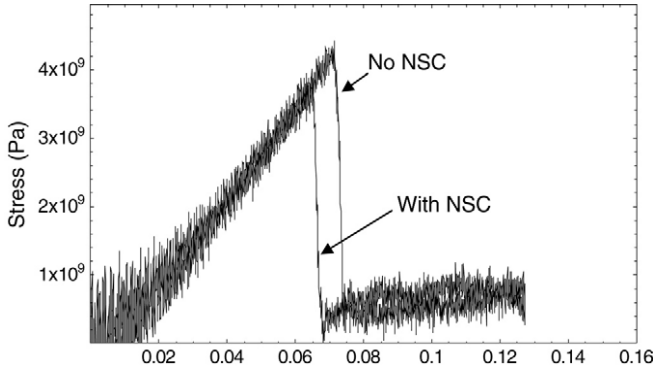

Fig. 13. Stress versus strain response for non-periodic boundary conditions and slow strain rate, straining case (iii). Two curves for the small crystal, i.e., for the intact one, and for the one with the NSC described in the text.

where short time scales (nanoseconds) force the study of very high strain rates and the small length scales in the atomistic simulation regions (usually from several thousand to several million atoms) may cause dislocation pile-ups and reflection of acoustic waves at the atomistic–continuum interface [33]. A detailed review of different approaches to the atomistic–continuum interface problem appears in [31]; in general, atoms fill in part of the FE mesh and usually coincide with a set of FE nodes. The contribution of the fill-in atoms to the total energy of the system is usually weighted in order to avoid overcounting of the energy at the interface.

For problems where inelastic deformation and crack nucleation/propagation is confined within "hot spots" of small spatiotemporal extent, concurrent FE/MD simulation techniques are feasible and provide great insight. Often, inelastic deformation and cracking is extensive so that its confinement within the spatiotemporal extent of computationally feasible atomistic simulations may not be possible. The simulation work reported herein illustrates this point: for example, see Fig. 9. Up to about the peak strength, deformation-induced atomistic defects are confined mainly in the area of the NSC. Yet, immediately at or slightly after the peak strength, long-range atomistic defects, mainly in the form of dislocations and stacking faults form, which would be hard to account for if a continuum was attached next to the atomistic crystal. For problems involving extensive inelastic deformation and crack propagation, for example for studying the effects of NSCs on the overall ductility of the system, an intermediate (between FE and MD) simulation technique may be appropriate, and kinetic Monte Carlo (kMC) is such an efficient technique. The kMC method is very well qualified to communicate effectively with both MD and FE, and is thus an excellent intermediate technique for handling problems where inelastic deformation and crack propagation extend beyond the immediate region of "hot spots". The time scales it can handle range from those in MD to those in FE, and the same holds for spatial scales. In [34] attempts to interface MC and MD techniques have appeared, while in [35] multiscale issues along the lines herein have been reported.

4. Conclusions

The following summarizes the major points advanced in this work.

- For Cu and for the straining cases and strain rates examined herein, the critical dimensions for the effects of NSCs are larger than the ones examined, i.e., up to 28.8 nm. Multiscale simulations are necessary to identify critical dimensions and also examine even slower strain rates.
- The spatial pattern of atomistic defects that develops during straining is different for a system with NSCs than one without NSCs. Yet, the number of atomistic defects (number of atoms with modified coordination number) seems to be independent of the NSCs. Samples larger than critical, simulated through periodic boundary conditions, tend to cluster atomistic defects.
- Surfaces are instrumental in initiating atomistic defects. Surface effects, also instrumental at macroscales, are beneficial at nanoscales, i.e., they significantly reduce the effects of stress concentrators. The absence of surfaces in the periodic boundary condition cases explains the observed increased strength for the intact crystals, and the high sensitivity to NSCs under periodic boundary conditions. Stress concentrations at the corners are not strong enough to drastically change this significant reduction of the effects of the NSCs.

- Strain rate (for up to one order of magnitude difference examined herein) does not alter the above conclusions.
- Computer power and experimental difficulties of the past did not allow one to speculate such an insensitivity to stress concentrators. Since stress concentrators play an important role in statistically assessing the strength and mechanical reliability of materials and structures, the results from the present study, should they ultimately prove true for every material, may shift the paradigm under which material reliability is studied for materials consisting of nanosize components, such as layered composites, for example.

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