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# The effects of stress concentrators on strength of materials at nanoscale: A molecular dynamics study

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## Abstract

There is evidence that when at least one spatial dimension of a material component is in the nanometer range, the effects of nanosize stress concentrators (NSCs) such as impurities, inclusions, pores, and cracks are either eliminated or significantly reduced. The aim of the paper is to examine such evidence using atomistic simulation techniques for a crystalline metal and identify the critical dimensions below which the effects of NSCs are minimal or even nonexistent. The preliminary results reported herein show that for Cu single crystals subjected to constant external strain rate, such critical dimensions are larger than about 30 nm. Since atomistic details are crucial in understanding material behavior at such scales, the paper points to the need for multiscale simulations techniques, presently being developed, for identifying critical dimensions and for examining slow strain rates. Based on the results, the paper presents simulation-based explanations why NSCs may be insignificant at nanoscales.

*Keywords:* Nano materials; Nano dimensions; Strength; Stress concentrators

## 1. Introduction

Materials show size effects, e.g., 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; Bazant and Chen (1997) cite 377 works on the subject mostly at scales from centimeters to several meters. A "simple" reasoning claims that larger-sized samples show a reduction in strength for probabilistic reasons: a larger sample simply has more flaws to initiate cracks. "Straightforward" reasoning suggests that as size approaches atomic dimensions, the theoretical material strength should be approached, and this

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has important applications within the context of nanoscience and nanotechnology, i.e., in developing nanostructural materials.

Any robust study of size effects must incorporate the defects in the material. Nanosize stress concentrators (NSCs) here indicate defects such as impurities, inclusions, cracks, pores; defects other than NSCs, e.g., dislocations, are also addressed yet they are considered part of the "bulk" material. NSC defects are present even in nanostructural materials, e.g., 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 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.

There is evidence that when at least one spatial dimension is below a critical one the effects of NSCs are either eliminated or significantly reduced; the evidence, as will be detailed in the sequence, suggests that such critical dimensions are in the nanometer range and, of course, depend on the material. Identification of such dimensions and material behavior at such scales will bring rigorous parameters in material design.

It is very interesting and relevant that the basic building components in many biological materials remarkable for their properties are at the nanoscale. It is very interesting that the basic building mineral crystal is in the nanoscale, i.e., the mineral thickness is normally several nanometers in bone, dentine, nacre (Wainwright et al., 1976; Rho et al., 1998; Jackson et al., 1988; Weiner et al., 1999; Smith et al., 1999; Kamat et al., 2000; Gao et al., 2003). One important yet to our knowledge unanswered question is: why the nanoscale? Some attempts to answer such an important question appear in Gao et al. (2003) on which some of the arguments in the following are based. It is also striking that such biological composites show consistency, particularly lack of crystallites or substructures above a certain size—after all, if this was not the case, defects would become increasingly important according to the thoughts advanced in this work. This consistency is particularly clearly seen in nacre and in enamel (Wainwright et al., 1976). In biological composites such as nacre, NSCs are protein molecules trapped within mineral crystals during biomineralization.

For engineering design purposes, size effects are one of the most compelling reasons for adopting fracture mechanics, which predicts a power law dependence of strength on size, with the exponent equal to $-1/2$, as opposed to classical strength of materials where the exponent is equal to zero (no size effect). Let us consider a piece of material containing a thumbnail crack, Fig. 1a. Based on the Griffith criterion, the failure strength of the film, $\sigma_{\mathrm{f}}$, under stress $\sigma$ is expressed as

$$\sigma_{\mathrm{f}} = a\sqrt{\gamma E/h} \tag{1}$$

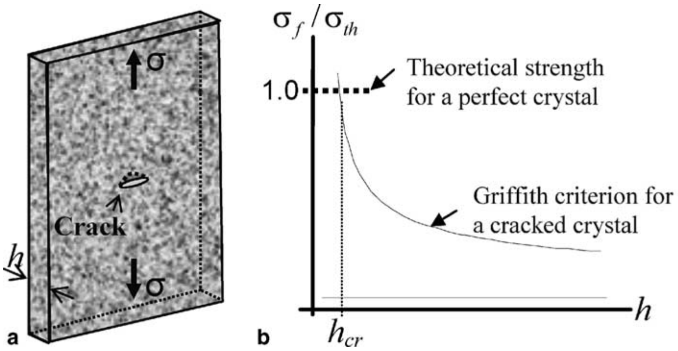

Fig. 1. (a) A small piece of material, a film or of a tube, of thickness $h$ containing a thumbnail crack-like defect subjected to stress $\sigma$. (b) Strength versus thickness plot, based on the Griffith criterion and schematic of the conjecture about $h_{\mathrm{cr}}$.

where $\gamma$ denotes the surface energy, $E$ the Young modulus, $h$ thickness (Fig. 1a) and $a$ depends on the crack geometry and is approximately equal to $\sqrt{\pi}$ for a thumbnail crack extending through half of $h$ and crack length equal to $h$. Fig. 1b shows schematically the plot of (1), where $\sigma_{\mathrm{th}}$ denotes the theoretical strength of the material (e.g. Hertzberg, 1996). Since $\sigma_{\mathrm{f}}$ cannot exceed $\sigma_{\mathrm{th}}$ a critical thickness, $h_{\mathrm{cr}}$ is conjectured (Fig. 1b). Considering rough estimates for a brittle material ($\gamma = 1\ \mathrm{J/m^2}$, $E = 100\ \mathrm{GPa}$, $\sigma_{\mathrm{th}} = E/30$ (Hertzberg, 1996) and $a = \sqrt{\pi}$) and using the Griffith criterion yields $h_{\mathrm{cr}} \approx 30\ \mathrm{nm}$ (Gao et al., 2003). Of course, there are several assumptions in this argument, especially if specialized for metals where the plastic deformation in the vicinity of the defect complicates the situation further. We note, for the sake of completeness, that crack-tip plasticity effects at such small (nano) scales may differ from those at larger scales as in "classical" elastic–plastic fracture mechanics. It is one of the goals of the present work to shed light in these assumptions as well as on the extension of the Griffith criterion to nanometer scales using simulations.

## 2. Simulation results on the effects of NSCs

We have performed simulations on single Cu(001) crystals with and without NSC defects in order to address the conjecture described above. The embedded atom method (EAM) for molecular dynamics (MD) simulations was employed; the applicability of 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 (cells) to be solved but impose an unneeded complication to the problems herein. The EAM (Daw and Baskes, 1984; Daw and Baskes, 1983; Daw, 1989) 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 (Plimpton and Hendrickson, 1993) modified for the purposes herein were performed on an HP super computer, i.e., using 64 EV-7 processors. Two sizes of three-dimensional crystals were simulated, one of size $28.8 \times 28.88 \times 28.88\ \mathrm{nm^3}$ ($x, y, z$, 2,048,000 atoms, thereafter termed as the "large") and one of size $18.05 \times 18.05 \times 18.05\ \mathrm{nm^3}$ ($x, y, z$, 500,000 atoms, thereafter termed as the "small"). In addition to straining the perfect crystals, the small and large crystals containing a NSC of $3.0 \times 3.0 \times 0.4\ \mathrm{nm^3}$ ($x, y, z$) positioned at their center were strained as well. In all simulations the $x$–$y$–$z$ crystal was strained in the $z$-direction (tensile straining) by fixing the atoms in the lower $z$ border plane and by imposing constant velocity on the atoms in the upper $z$ border plane. The imposed velocity was such that the strain rate was $10^9\ \mathrm{s^{-1}}$; the issue of strain rate is discussed in the sequence.

Fig. 2 shows simulation of tensile strain rate imposed on the large crystal containing the flat NSC oriented transverse to the loading direction. Up to about the peak strength, deformation induced atomistic defects (atoms for which the coordination number changed during deformation) 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. Fig. 3 shows the results for the same crystal as that in Fig. 2 yet without the NSC. As expected, the crystal without the NSC forms isolated slip planes (111) while in the one with the NSC several slip planes form. Even though the NSC is a dislocation 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 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 the NSC; for compactness, the graphs are not shown herein.

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 is rather independent of the presence of the NSC for

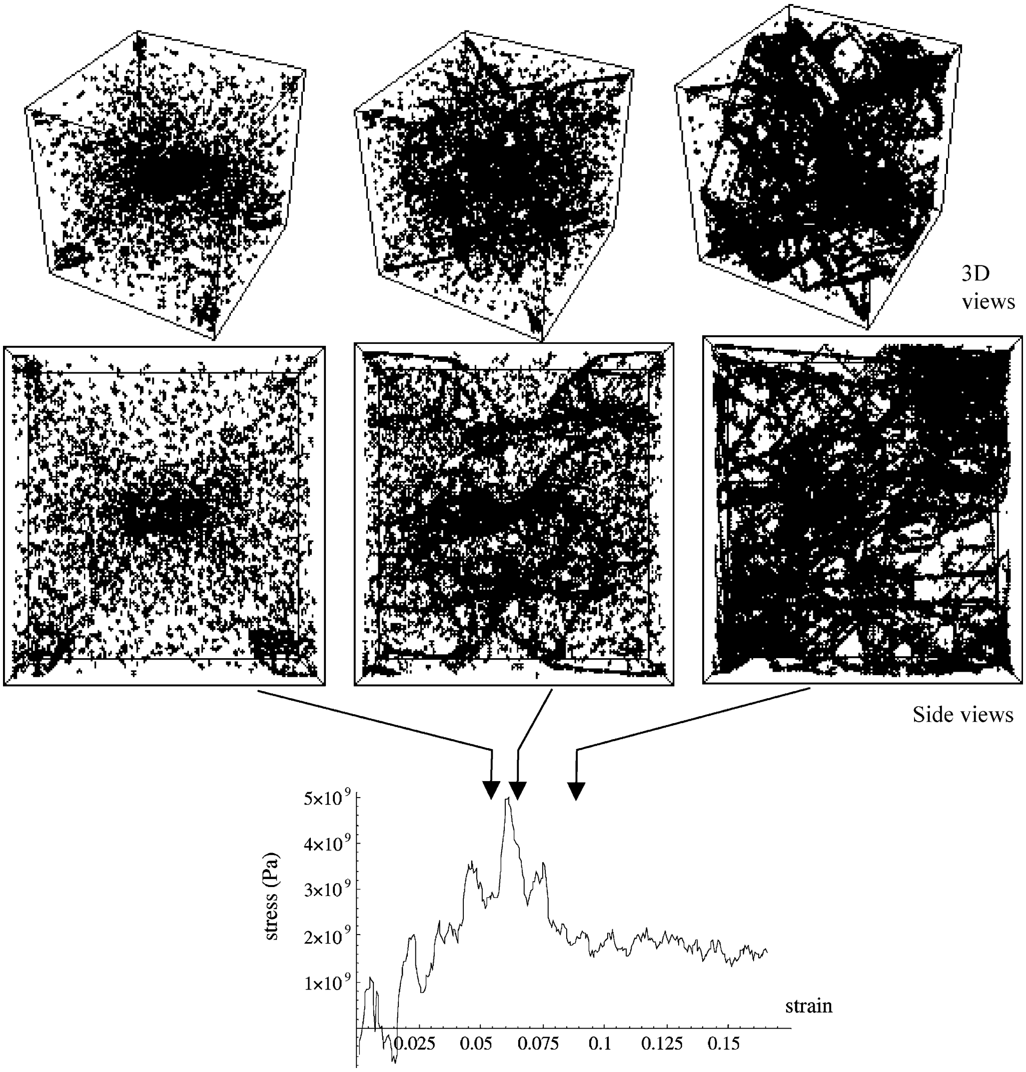

Fig. 2. Simulation of tensile strain rate imposed on a Cu(0 0 1) single crystal, $28.88 \times 28.88 \times 28.88\,\mathrm{nm}^3$ (2,048,000 atoms). The otherwise perfect crystal contains a $3.0 \times 3.0 \times 0.4\,\mathrm{nm}^3$ NSC (pore/crack) at its center, and tensile load is imposed in the vertical direction. The graph shows the stress–strain response. The six figures show atoms of which the coordination number changed from that of the perfect crystal during deformation. Top row: 3D views at strain of 0.055, 0.065, and 0.085, respectively. Bottom row: side views at strain of 0.055, 0.065, and 0.085, respectively.

the cases examined, as shown in Fig. 4. Naturally, the question why this independence of the stress versus strain response on the presence or lack thereof of the NSC comes up. In this paper, the purpose of which is to present some rather preliminary results on the subject, some “answers” to this intriguing question are offered. Yet, the need for extensive theoretical and experimental work is pinpointed. We hope that this communication will trigger further investigations by several researchers.

Fig. 5 shows that the number of atomistic defects (number of atoms with modified coordination number) is rather independent of the presence of the NSC; a similar plot was obtained for the large crystals. An explanation for this is that the large surface to volume ratio of these nanosystems is instrumental in

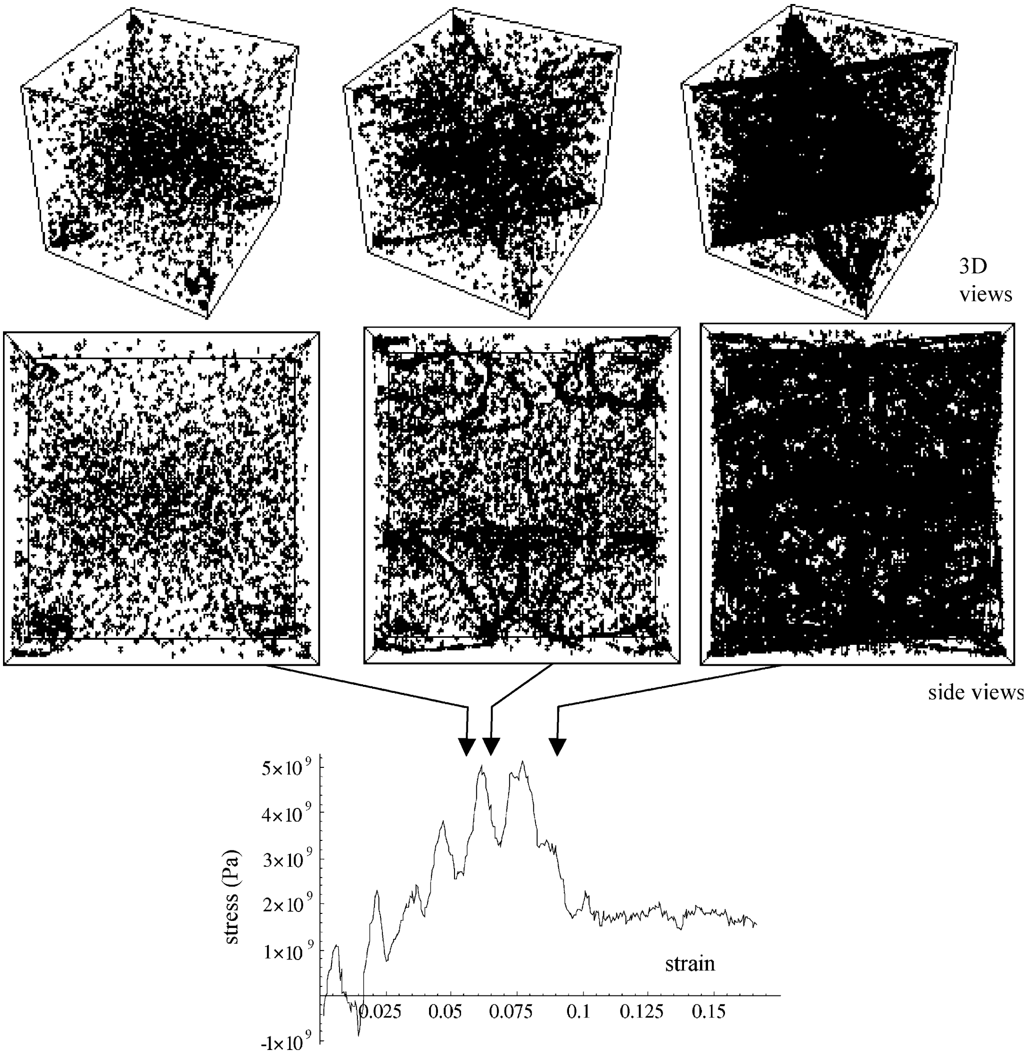

Fig. 3. Simulation of tensile strain rate imposed on a Cu(0 0 1) single crystal, 28.88 × 28.88 × 28.88 $\text{nm}^3$ (2,048,000 atoms) without any NSC. Tensile load is imposed in the vertical direction. The graph shows the stress–strain response. The six figures show atoms of which the coordination number changed from that of the perfect crystal during deformation. Top row: 3D views at strain of 0.055, 0.065, and 0.085, respectively. Bottom row: side views at strain of 0.055, 0.065, and 0.085, respectively.

initiating atomistic defects. If, on average, the energy required for forming each atomistic defect is constant, this explains insensitivity of the material to NSCs.

## 3. Conclusions

For Cu subjected to tensile strain at the examined strain rates ($10^9\ \text{s}^{-1}$), the critical dimensions for the effects of NSCs are larger than the examined (up to) 28.8 nm. Multiscale simulations are necessary to identify critical dimensions and also examine slower strain rates.

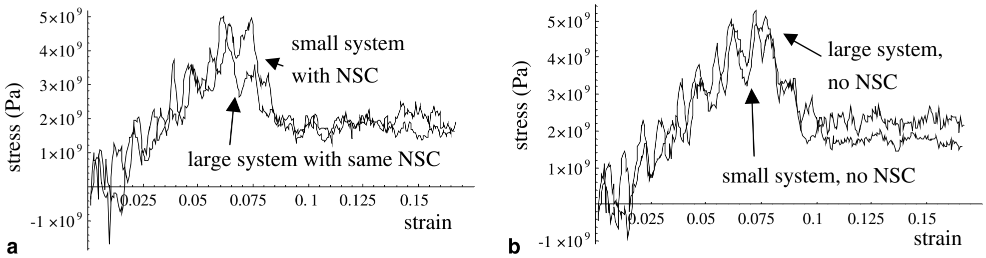

Fig. 4. Stress versus strain curves for four systems: (a) small and large system with same size NSC; (b) small and large system without any NSC.

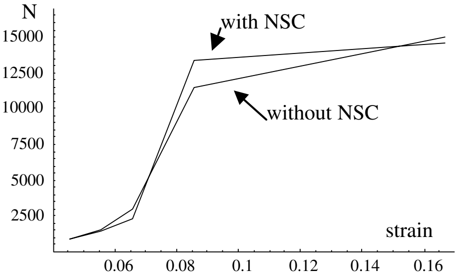

Fig. 5. Total number of atomistic defects, *N*, versus strain for the small Cu(001) system with and without NSC. Plot was obtained from atom positions at five strain levels during deformation.

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) is rather independent of the NSCs. If, on average, the energy required for forming each atomistic defect is constant, this explains insensitivity of the material to NSCs. However, such atomistic defects should not be spatially clustered for this argument to be valid. Even though this is the case in the simulations reported herein, it will be interesting to study clustering of defects in larger samples, especially larger than the critical size conjectured herein.

The large surface to volume ratio of these nanosystems is instrumental in initiating atomistic defects. Thus, surface effects, also instrumental at macroscales, are beneficial at nanoscales, i.e., they eliminate the effects of stress concentrators. Computer power and experimental difficulties may have not allowed speculating such an insensitivity to stress concentrators in the past. 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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