Analysis of surface effects on the deformation of a nanovoid in an elasto-plastic material

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A B S T R A C T

Surface effects, usually embodied as surface tension or surface energy, become considerable in nanostructured materials. With attention to static finite deformations, we present a theoretical analysis about the surface energy effects on the evolution of a nanovoid in a plastic material. The following improvements have been incorporated based on the previous studies: (a) the initial configuration is assumed to be the equilibrium state, which is reached by applying the surface tension onto a fictitious stress-free configuration; (b) both cases of applying compressive and tensile hydrostatic stress is discussed. This illustrative solution provides some reasonable physical interpretations of the following "unconventional" phenomena: (a) when the void radius is smaller than some critical value, finite plastic flow happens in the process from the fictitious stress-free configuration to the initial configuration, which will dramatically influence the subsequent responses; (b) size effects exist, i.e., the growth of nanovoids is closely related to their sizes; (c) the tension–compression asymmetry becomes stronger with decreasing the void size; (d) void shrinkage instability can arise.

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1. Introduction

Deformations of voids on the nanometric scale are studied with the consideration of surface energy, whose importance has been widely recognized [1,2]. The main characteristic of this study is to consider the prehistory elasto-plastic deformation caused by the surface energy on the void surface, during the investigation of its response under external loadings.

1.1. A brief literature review on surface effects

Surface effects in the mechanics of nanostructured elements, including nanoparticles, nanowires, nanobeams, nanofilms and materials containing nanoscale inhomogeneities such as cavities, have attracted considerable research attention, e.g. [1,3]. Here, we focus on the basic concepts of surface tension and composition as related to growth of nanovoids in plastic materials.

The first two concepts are surface tension and surface energy. The idea of surface tension is proposed by Cabeo [4] and is stated more explicitly by Segner [5]. Shuttleworth [6] derives the relationship between surface tension and surface energy. We adopt his definitions in this research: "The surface energy is the work necessary to form unit area of surface by a process

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of division; the surface tension is the tangential stress (force per unit length) in the surface layer; this stress must be balanced either by external forces or by volume stresses in the body". Zhou and Huang [7] and Tang et al. [8] argue that the surface tension depends on the competition between electron redistribution and the lower coordination on surfaces. For simplicity, the surface tension and surface energy are assumed to be constant in the present analysis, and commonly denoted by γ, which has values 0–5 N m^{-1} for most metals as shown by Vitos et al. [9].

Another important concept, the atomic structure of the surface, also deserves attention. From an atomistic viewpoint, it is actually a surface layer within a few atomic spacings of the outmost surface atom layer [6]. For example, molecular dynamics (MD) simulations were used by Diao et al. [10] to model the free relaxation process of a gold nanowire from a fictitious unrelaxed configuration to a physically realistic configuration. The outmost two layers of atoms decrease upon relaxation. The formation of such a layer is driven by unequilibrium interatom forces arising when a new surface is made, for instance, by cutting operation. Furthermore, plastic deformation in nanostructured elements under external loadings will generally change the density and number of the atoms at a surface [3]. Processes of surface formation and deformation are complicated and usually associated with atomic rearrangement. Nevertheless, this complexity adds no difficulty to the current study because surface tension (energy) is in principle a continuum-type concept. The value of surface energy is largely dependent on the atomistic spacing in the surface layer. For metals, finite deformations are mainly achieved by dislocations instead of changes in atomistic spacing. Thus, we assume the constant atomistic spacing and therefore the constant surface energy in the finite deformation processes in metals.

The last concept is the specific surface area (SSA), namely the ratio of the surface area to the volume of the bulk [11]. The high SSA value of nanostructured materials is generally considered to be the cause for their mechanical behaviors, which can be very different from the behaviors of the macro-bulk. This conclusion is true for nanofilms, nanowires, nanobeams and nanoparticles, but is not true for nanovoids because the SSA value is close enough to zero when a nanovoid is embedded in infinite bulk materials. The unique characteristic of nanovoids is that the bulk is outside of the void surface, unlike in nanoparticles in which the bulk is surrounded by its surface. Instead of revisiting detailed studies on effects of the SSA in the fields of materials science and mechanics [3], here we reflect its association to Torricelli's trumpet, an "unthinkable" idea first observed by Evangelista Torricelli, a student of Galileo [12]. This trumpet has a finite volume, $V = \pi$, but an infinite surface area, $S = 2\pi \ln x|_1^\infty = \infty$. This can be only mathematically true. Actually, this infinite surface cannot be manufactured in the real physical world. If we consider that everything is composed of atoms, the maximum surface area will reach $S = 2\pi \ln x|_1^{10^{10}} = 20\pi ln\, 10$ if the atom radius is equal to 10^{-10} m. By the way, there is a continuous increase in SSA along the length of the trumpet and it can be a potential idea for making a functionally graded material. The purpose of mentioning the Torricelli's trumpet is to show the atomic composition nature of materials, because it becomes crucial for accurate descriptions of material composition especially at the nanometer level. The above reflection on Torricelli's trumpet indicates that mathematics and physics do not always coincide with each other, and should be a note on the Gibbs idealization [13] describing the surface layer as a "mathematical surface" with a zero thickness, as well as the feasibility of continuum theories, which is questioned by some researchers such as Huang et al. [14]. Although the present study is conducted within the continuum framework, the validity of continuum concepts deserve a great awareness.

Nanovoids with the surface effects have been studied intensively in the elastic regime. Yang [15] discusses the effective bulk and shear moduli of heterogeneous materials containing spherical nanovoids at dilute concentrations. Duan et al. [16] discover that nanoporous materials can be made stiffer than non-porous counterparts by surface modification. He and Li [17] examine the effect of surface stress on stress concentration near a spherical void in an elastic medium in the framework of continuum surface elasticity. Unfortunately, these theoretical works are confined to systems of simple geometry, therefore numerical simulation techniques have also been widely applied to more complex geometries. For example, Wei et al. [18] study the size-dependent mechanical properties of nanostructures by developing a kind of surface element to take into account the surface elastic effect. Chen et al. [11] propose a continuum model by introducing the surface energy to the total potential energy, then implement the model using the finite element method.

To date, plastic deformation with the inclusion of nanovoids has been studied much less compared with the elastic response, mainly because both surface atom rearrangements and atom exchange can occur during finite plastic deformations. Some efforts in this area have been made within the framework of continuum mechanics. Within the small deformation regime, Zhang et al. [19] study the plastic deformation of nanoporous materials and nanocomposites with consideration of both the surface residual stress and the surface elasticity. Huo et al. [20] assume a constant surface energy and study its effects on the growth of a spherical shell or a thick cylindrical column, concluding that for typical metals, the surface effect is negligible for voids larger than 100 nm, but it becomes significant when the void size is on the order of 10 nm. Considering the size effect due to the plastic strain gradient which becomes important from hundreds of microns to hundreds of nanometers, Gao et al. [21] and Huang et al. [22] propose the mechanism-based strain gradient plasticity and then use this theory to solve the void growth problem. Nevertheless, the strain gradient effect is not possible to increase unlimitedly with decreasing the characteristic size of plastic deformation. For example, Bažant [23] addresses that the questionable small-scale asymptotic behavior can exist. That is why the concept of maximum allowable dislocation density has been later mentioned [24,25]. Based on this fact, we are not going to consider the gradient effect because we argue that the surface effect is more dominant than the gradient effect when the void size is smaller than 20 nm. We admit this ignorance makes the result somehow less accurate, but we would say that the bottom line is that the tendencies found in this study is qualitatively