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On the conical indentation response of elastic auxetic materials: Effects of Poisson's ratio, contact friction and cone angle

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ABSTRACT

The linear elastic analytical solution of an axisymmetric probe indenting a semi-infinite half-space forms the backbone of most indentation data analysis protocols. It has been noted in the literature that the theoretical solution relies on a boundary condition that is ill-posed which leads to discrepancies from the actual response that depends, among other parameters, on the Poisson's ratio of the indented material. While correction factors have been proposed, prior studies have concentrated on the positive Poisson's ratio regime and have neglected an exciting and developing class of materials: the auxetic systems. The finite element method is used to simulate the conical indentation response of elastic materials with Poisson's ratios covering the whole thermodynamically possible range, $-1 \leq \nu \leq 0.5$. Consistent with theoretical predictions, the indentation resistance and hardness of auxetic materials is enhanced compared to their non-auxetic counterparts. The stress profiles and contact details are systematically analyzed and the increase in resistance is traced to the shear stiffening and the reduction of contact area compared to conventional materials. Furthermore, it is shown that the analytical linear elastic solution falls short in accurately describing the indentation response, especially for negative Poisson's ratio materials. In contrast to the theoretical prediction, the contact area reduces as the Poisson's ratio increases resulting in increased required force to penetrate the material and an enhanced pressure distribution beneath the indenter. The analytical solution is corrected for the whole ν range and best fit polynomials are proposed for ease-of-use. The effects of contact-friction and indenter cone-angle are also studied and quantified.

1. Introduction

Instrumented indentation has developed into a standardized tool for nano- and micro-mechanical characterization of materials (Bulychev et al., 1975; Doerner and Nix, 1986; Fischer-Cripps, 2002; Oliver and Pharr, 2011,1992). It was initially introduced for characterizing thin films and sub-micron material volumes but it has expanded its application range into studying virtually all classes of material systems: metals (Schuh, 2006; Tabor, 2000), ceramics (Cook and Pharr, 1990; Lawn, 1998; Wachtman et al., 2009), polymers (Tweedie et al., 2007; Vandamme et al., 2012; VanLandingham et al., 2001) and composites (Constantinides et al., 2009, 2006, 2003; Němeček et al., 2013).

The current state of hardware and electronics ensures that loads and displacements can be recorded with nN and angstrom scale resolutions, respectively, and force-displacement curves are nowadays routinely collected either in the nanometer or micrometer regime. An equally important step in the nanomechanical characterization of materials is the conversion of experimental data into meaningful material properties. There are several analytical approaches for completing this step most of which have focused on the indentation modulus ($E*$) and hardness (H) of the material:

$$E^* = \frac{\sqrt{\pi}}{2}\frac{S}{\sqrt{A_c}} \tag{1}$$

$$H = \frac{P_{\max}}{A_c} \tag{2}$$

where S is the unloading slope at maximum depth ($h_{\max}$), $S = dP/dh|_{h_{\max}}$, A_c is the area of contact at maximum load ($P_{\max}$). $E*$ and H, under certain circumstances, can be converted to the elastic modulus (Borodich and Keer, 2004a, 2004b; Pharr et al., 1992) and strength characteristics (Cariou et al., 2008; Ganneau et al., 2006; Tabor, 2000) of the indented system. In the case of a rigid indenter $E*$ relates to the plane stress modulus of the material, $E^* = \frac{E}{(1-\nu^2)}$

Directly or indirectly most analysis methods make use of the analytical solution of an axisymmetric indenter being pushed against a semi-infinite, linear elastic half-space. In fact Eq. (1) can be directly

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derived from the linear elastic solution (Bulychev et al., 1975; Oliver and Pharr, 1992) and it has been proven that it holds true for any indenter that can be described as a solid of revolution (Pharr et al., 1992). Impressively enough, the equation is still valid even if the material exhibits elastic–plastic response with the only provision that the area of contact is properly accounted for in the analysis (Cheng and Cheng, 1997). In other words all plasticity phenomena are incorporated into the area of contact and provided that this is accurately captured, Eq. (1) continues to hold.

Several finite element studies (Bolshakov and Pharr, 1998; Cheng and Cheng, 1999, 1998; Dao et al., 2001; Troyon and Huang, 2011) have pointed out that computational results deliver consistently higher values of the modulus of elasticity when calculated through Eq. (1). A detailed analysis by Hay et al., (1999) in her, by now, classic paper of 1999 has deciphered the origins of this discrepancy which has its roots on an inaccurate boundary condition used in the formulation of the mathematical problem that has been analytically solved (see Section 2); the issue of tangential displacements has also been reported in several other studies (Argatov, 2004; Kindrachuk et al., 2009), see also discussion and references in Borodich (2014)). Through finite element modeling they have quantified this uncertainty and they have formulated analytical approximations for a correction factor γ for Eq. (1) based on simple modifications of Sneddon's solution, which proved to be a function of Poisson's ratio of the material (ν) and the cone semi apex angle (θ):

$$E^{*} = \frac{1}{\gamma}\frac{\sqrt{\pi}}{2}\frac{S}{\sqrt{A_c}} \tag{3}$$

$$\gamma = 1 + \frac{\beta}{4\tan\theta} \tag{4}$$

$$\gamma = \pi\frac{\frac{\pi}{4} + 0.15483073\cot\theta\frac{\beta}{4}}{\left(\frac{\pi}{2} - 0.83119312\cot\theta\frac{\beta}{4}\right)^{2}} \tag{5}$$

where $\beta = \frac{1-\nu}{1-2\nu}$. Eq. (4) is best suited for cube-corner indenters whereas Eq. (5) for Berkovich/Vicker-type geometries. While correction factors have already been proposed (Hay et al., 1999; Poon et al., 2008; Xu, 2008), the majority of studies (with a few recent analytical exceptions (Argatov and Sabina, 2014; Argatov et al., 2012) have concentrated in the positive Poisson's ratio regime and have neglected an exciting and developing class of materials: the auxetic systems. The thermodynamic constrains on the materials elastic properties allow for Poisson's ratio of the material to move into the negative domain, more specifically $-1 \leq \nu \leq 0.5$. This leads to the counter-intuitive behavior, in which materials tend to expand in the lateral dimension in response to stretching. This geometrically/kinematically-driven response to loading leads to an increase in volume and thus materials that fall into this category have been termed auxetic. Equivalently the same materials will tend to reduce their volume when compressed (thus miotic). Ever since the experimental reporting of such a response by re-entrant structures polyurethane in 1987 by Lakes (1987), many other systems have been found to exhibit similar deformation patterns. Most of these systems fall into man-made or naturally occurring microporous systems like polytetrafluoroethylene (Lakes, 1987), microporous ultra high molecular weight polyethylene and polypropylene (Alderson et al., 2000, 1994), various types of rocks and crystals (Zouboulis et al., 2014), a-cristobalite (Grima et al., 2005), zeolites (Gatt et al., 2008), various laminate composites (Milton, 1992), defected graphene (Grima et al., 2015), and many others. For a more detailed exposition of this particular material behavior the reader is referred to the reviews of Lakes (1993), Yang et al. (2004) and Greaves et al. (2011).

The finite element method is used in this paper to simulate the conical indentation response of elastic materials with Poisson's ratios covering the whole thermodynamically possible range, $-1 \leq \nu \leq 0.5$. The aim of this particular study is twofold: on one side we aim to quantify the increased indentation resistance reported in the literature when indenting auxetic materials and identify through computational simulations the mechanisms that lead to this particular response. On the other hand we aim to deal with the discrepancy caused by the existing analytical solution when indenting auxetic materials and extract correction factors that will eliminate any inaccuracies and will correct the analytical solution for the entire possible span of Poisson's ratios.

2. Theoretical background

The main focus of contact mechanics is the determination of size and exact shape of the contact area. Unlike classical mechanics problems, the contact zone is unknown so that areas where displacements (in the contact region), and those where forces (free surface) are prescribed are not known *a priori*. This renders the analysis intrinsically non-linear, since the surface boundary conditions have to be formulated under restrictions of a point z that is either situated in the contact zone or in the stress-free area. The contact problem between a rigid axisymmetric indenter and an infinite half-space is described by the following set of equations, written in polar coordinates (ρ, φ, z):

$$div\,\sigma = 0 \tag{6}$$

$$\sigma = F(\varepsilon) \tag{7}$$

$$\varepsilon = \frac{1}{2}\left(\nabla u + \nabla^{t} u\right) \tag{8}$$

$$P = -\int_{\rho=0}^{a}\int_{\theta=0}^{2\pi}\sigma_{zz}(\rho,\varphi,0)\rho d\rho d\varphi \tag{9}$$

$$u_z(\rho,\varphi,0) = -h + f(\rho);\ \rho < \alpha \tag{10}$$

$$\sigma_{\rho z}(\rho,\varphi,0) = 0;\ \rho > 0 \tag{11}$$

$$\sigma_{zz}(\rho,\varphi,0) = 0;\ \rho > a \tag{12}$$

where P is the applied load, in direction z, $f(\rho)$ defines the axisymmetric shape of the indenter, and a is the contact radius. Eq. (6) is the static equilibrium condition, Eq. (7) provides the stress–strain relation of the indented material (here linear isotropic elastic), Eq. (8) links strain to displacements and the remaining relations (Eqs. (9)–(12)) are the boundary conditions for the total load (Eq. (9)), the vertical displacement in the contact region (Eq. (10)), the zero shear stress on the surface (Eq. (11)) which includes the frictionless contact condition and the stress-free boundary condition outside the contact zone (Eq. (12)).

There are several ways of solving the above set of equations, the more traditional one being the method developed by Lee and Radok (1960), and further formalized by Sneddon (2010) and (1965) which consists in performing on all problem equations two dimensional Fourier transforms in the directions of the surface coordinates x and y. In the case of axi-symmetry, this integral transform is called a Hankel transform on the polar coordinates ρ and φ which are transformed into a variable φ of dimension L^{-1}. The area of contact is circular by symmetry and its projected radius a is kept as an unknown. It turns out that the equations written with a new set of non-physical coordinate can be solved analytically in the transformed space. Finally the integral transforms are performed backwards to return to the original problem. Following this procedure, the expressions for h and P for an isotropic half-space read:

$$h = \alpha\int_{\rho=0}^{\alpha}\frac{f'(\rho)d\rho}{\sqrt{a^{2}-\rho^{2}}} \tag{13}$$

$$P = 2\frac{E}{1-\nu^{2}}\int_{\rho=0}^{\alpha}\frac{\rho^{2}f'(\rho)d\rho}{\sqrt{a^{2}-\rho^{2}}} \tag{14}$$