ARTICLE IN PRESS

International Journal of Plasticity xxx (2016) 1–25

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

Large elastoplasticity under static megabar pressures: Formulation and application to compression of samples in diamond anvil cells

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ARTICLE INFO

Article history:
Received 14 December 2015
Received in revised form 29 April 2016
Available online xxx

Keywords:
B. Elastic-plastic material
B. Finite strain
C. Numerical algorithms
B. Constitutive behaviors

ABSTRACT

In high pressure research, static megabar pressures are typically produced by compression of a thin sample by two diamonds in various types of diamond anvil cells. This process is accompanied by large plastic deformation (sample thickness is reduced by a factor of 30), and finite elastic deformation of a sample and even the diamond. A thermodynamically consistent system of equations for large elastic and plastic deformation of an isotropic material obeying nonlinear elasticity and pressure dependent yield condition is formulated. The Murnaghan elasticity law and pressure-dependent J_2 plasticity are utilized. The finite-strain third-order elasticity law for cubic crystals is utilized for diamond. A computational algorithm is presented with emphasis on the stress update procedure and derivation of the consistent tangent moduli. It is implemented as a user material subroutine in the finite element code ABAQUS. Material parameters for a rhenium sample, as an example, and a diamond are calibrated based on the experimental and atomistic simulation results in the literature. The evolution of the stress and strain tensor fields in the sample and diamond is studied up to a pressure of 300 GPa. Good correspondence between numerical and experimental pressure distributions at the diamond-sample contact surface is obtained. Because there is a significant scatter of the magnitude of reported third-order single-crystal elastic moduli for diamond, their effect on strains and stresses is studied in detail. With the smaller third-order elastic moduli, the phenomenon of cupping of the diamond-sample contact surface is reproduced, which plays an important role in increasing maximum pressures for a given anvil geometry. The results provide important insight into the mechanical response in diamond anvil cells, interpretation of materials properties under extreme conditions from heterogeneous fields, and optimum design of cells for reaching the maximum static pressure in a volume sufficient for the desired measurements.

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http://dx.doi.org/10.1016/j.ijplas.2016.04.017
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Please cite this article in press as: Feng, B., et al., Large elastoplasticity under static megabar pressures: Formulation and application to compression of samples in diamond anvil cells, International Journal of Plasticity (2016), http://dx.doi.org/10.1016/j.ijplas.2016.04.017

1. Introduction

The behavior of materials under high pressures is of great fundamental and applied interest. Fundamental aspects concern the search of new materials, phenomena, and unique properties that appear under extreme conditions. The interior of each planet is under high pressure; thus, geophysical research is heavily based on the study and interpretation of a material mechanical, physical, and chemical behavior under high pressure. Applied aspects include transforming high-pressure discoveries in technology, *e.g*., industrial synthesis of diamond and cubic boron nitride (Novikov, 2005).

From the mechanical point of view, the main questions are: how it is possible to produce pressures exceeding by two orders of magnitude the yield strength of the sample and more than an order of magnitude the ultimate strength of the tool (anvils) used to produce high pressures. Both issues can be addressed by considering plastic compression with large strains of a thin sample between two anvils with a conical part. Plastic compression of a sample in the presence of friction shear stresses at the contact surface between the sample and anvils corresponds to the classical Prandtl problem (Hill, 1950) on compression of a perfectly plastic thin layer or its approximate axisymmetric solution, which is broadly used in metal forming (Eremets, 1996; Hill, 1950; Levitas, 1996; Thomsen et al., 1965). It is described by the simplified equilibrium equation and its solution

$$\frac{dp}{dr} = -2\tau_f \Big/ h; \;\; \tau_f = \tau_y \approx 0.5\sigma_y \rightarrow p = p_R + \sigma_y (R-r)\big/h, \tag{1}$$

where p and p_R is the pressure at radii r and R, respectively, h is the thickness of the thin layer, and τ_f is the shear friction stress at the contact surface. For a thin sample (large R/h), friction stress τ_f in the major part of the contact surface reaches its maximum value when it is equal to the yield strength in shear τ_y, which is taken into account in Eq. (1). For small sample thickness h and large yield strength in compression $\sigma_y \approx 2\tau_y$, a very large pressure gradient develops. Thus, the pressure at the center exceeds pressure at the edge of a sample R, p_R, by $\sigma_y R/h$, *i.e*., for large R/h it can be large as well. A large pressure gradient over the relatively small working area of an anvil along with the conical shape of an anvil (the principle of massive support as developed by Bridgman, 1952) allows an anvil to carry such high stresses in a small volume surrounded by a less stressed volume. Of course, the larger the yield strength of a sample (or gasket, in a hole of which the sample is placed), the higher the pressure can be achieved; the larger the strength of an anvil, the higher the pressure can be produced without fracture of an anvil.

Experiments for studying the material properties and transformations under the static pressure of several megabars are routinely produced in various types of diamond anvil cells. The characterization of anvils under those conditions have been examined in early studies by Hemley et al. (1997), Mao and Bell (1978), and Moss et al. (1986). These studies showed that the determination of stress-strain fields in both diamond and a sample/gasket is of vital importance. For complete characterization of the properties and transformations one needs to know fields of all components of the stress, and elastic and plastic strain tensors, both in a sample and diamond. Stress and strain fields in diamond anvils are required for their optimal design, preventing fracture, and reaching maximum possible pressure. In early treatments, the pressure distribution along the contact surface between a sample and diamond was measured (Goettel et al., 1985; Hemley et al., 1997; Jeanloz et al., 1991; Levitas et al., 2006; Meade and Jeanloz, 1988; Novikov et al., 1991a; Sung et al., 1977; Vohra et al., 1988; Weir et al., 1998). This distribution combined with the measured sample thickness under the load was used to determine the pressure dependence of the yield strength in shear (Jeanloz et al., 1991; Levitas et al., 1996; Sung et al., 1977; Weir et al., 1998; Zhao and Zhang, 2007), which in the major part of the contact surface is equal to the shear friction stress. Other studies in more recent works included obtaining experimental constraints on the components of the elastic strain tensor that have been measured in some selected regions of a sample using axial or radial X-ray diffraction (Duffy et al., 1999b; Hemley et al., 1997; Hemley et al., 2005; Merkel et al., 2013; Nisr et al., 2014; Singh, 1993; Singh et al., 1998, 2012; Wenk et al., 2007). If the pressure-dependence of the elastic moduli of a single crystal is known, stresses can be calculated. For polycrystalline samples, additional assumptions that allow connecting single and polycrystalline elastic moduli (*e.g.* Hashin-Shtrikman) are required for proper treatments. In this respect, methods have been developed to measure the distribution of elastic lattice strains that are used to obtain distribution of stresses (Merkel et al., 2013; Nisr et al., 2014; Wenk et al., 2007).

Numerical methods for determination of stress and strain fields have also been developed and applied to modeling different high pressure devices. Solutions for the stress state of perfectly plastic material in different high pressure apparatuses (including Bridgman anvils) with different geometries have been obtained using slip-line methods. These devices include those employing Bridgman or diamond anvils, recessed anvils used for diamond synthesis, toroidal types of anvils, and belt apparatuses (see Levitas, 1981, 1996) and textbook by Eremets (1996). Strain state and plastic flow have not been considered in these methods and the anvils were in general considered to be rigid. Finite element method (FEM) simulations of the stress state of different types of anvils, including recessed anvils (Novikov et al., 1986), belt type devices (Levitas et al., 1986), and diamond anvils (Novikov et al., 1987), have been performed, where boundary conditions were taken from the slip-lines solutions. Strength and durability criteria for cemented carbide (Novikov et al., 1986, 1991b; 1991c, 1991d) and diamond anvils (Novikov et al., 1987, 1992, 1994) were suggested, including size effects, and optimization of anvils based on this criteria, has been developed. Notably, the criterion of maximum elongation orthogonal to the cleavage plane was found to be justified for diamond for relatively low pressure (Voronin et al., 1984). Other FEM approaches (Adams and Shaw, 1982; Bruno and Dunn, 1984) have studied stress distributions resulting from various beveled angles, where boundary conditions were schematized rather than strictly determined, and both metal gasket and diamond were generally treated as isotropic elastic materials.

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