Tensorial stress–strain fields and large elastoplasticity as well as friction in diamond anvil cell up to 400 GPa

Valery I. Levitas1,2*, Mehdi Kamrani3 and Biao Feng4

INTRODUCTION
In static high-pressure research, megabar pressures are generated by compression of a thin sample by two diamonds in diamond anvil cells (DAC)1–4, see Fig. 1. This process is accompanied by large plastic deformation of a sample and large elastic deformation of the diamond.5,6 Various problems, such as the study of physical, chemical, geological, and mechanical phenomena and synthesis of new phases in a sample, as well as the increasing range of achievable pressures,1–23 are related to knowledge of the fields of all components of the stress, elastic, and plastic strain tensors in DAC. While most measurements and discussions are related to pressure only, it is evident that elastic deformation and fracture of diamond and plastic flow of a sample and gasket depend on all components of the stress tensor. Contact friction between diamond and sample/gasket plays a key role in generating high pressure without fracture of the diamond; friction is a shear stress that depends on the stress normal to the contact surface. It is also well-known that phase transformations and chemical reactions in solids depend not only on pressure, but also on the deviatoric stresses and plastic strains.12,14–16,20–23 All of these fields are extremely complex and heterogeneous, e.g. with normal stresses varying by megabar over 20 μm.6,7

Measurement of the radial pressure distribution at the sample–diamond boundary was based on the ruby fluorescence method, which worked up to 185 GPa.5 For higher pressure, radial pressure distribution averaged over the sample thickness is determined using X-ray diffraction in a sample.5,7 The radial thickness profile, which characterizes both elastic deformation of an anvil and elastoplastic deformation of a sample/gasket, was measured utilizing in situ high-pressure X-ray absorption.5,7 Measurement of the deviatoric stress was limited to the difference between axial stresses $\sigma_{zz}$ and radial stresses $\sigma_r$ averaged over the entire sample.6,9,12–19 Plastic deformation fields in the sample compressed in DAC and contact friction stresses were not measured at all. Thus, despite significant progress, it is unlikely that all tensorial fields in DAC will be measured. Theoretical approaches and finite element method (FEM) simulations23–29 of the DAC are based on relatively simple models with linear pressure dependence of the yield strength and simplified contact friction conditions. The most sophisticated model and the best numerical reproduction of the experimental pressure distribution in ref. 5 was obtained in ref. 27 for compression of rhenium up to 285 GPa. However, in that study the plastic sliding along the contact surface and also the dependence of the friction coefficient on the normal contact pressure were ignored. Also, good correspondence was obtained for one pressure distribution only; for two smaller pressure levels, significant deviation from the experiment existed, i.e. the model is not adequate. To obtain such a description of the experiment, the third-order elastic constants of diamond were modified. Besides, since experimental thickness profiles of the sample were not available, reproducing the pressure distributions was aimed only. Thus, while essential improvement in reproducing pressure distribution in comparison with the previous works26,27 was achieved, obtained mechanical properties cannot be considered as verified, and corresponding stress and plastic strain tensor fields may contain significant inaccuracies.

We suggest the following coupled experimental—theoretical—computational approach for determination of all stress and plastic strain tensorial fields, elastoplastic properties, and contact friction rules. All fields that can be measured should be measured. Physics-based models for elastoplastic behavior and contact friction should be iteratively developed and refined, and all material properties should be calibrated by fitting to some experimental fields and verified by comparison with other experimental fields. With these properties, simulations provide all fields, including components of the stress and plastic strain tensors, friction stress, etc., i.e., those which cannot be directly measured. To obtain the first results from this method, we will use...
accumulated plastic strain

the postulate of the perfect plasticity that, above some level of

the friction coefficient $\tau$

plasticity provides adequate description of experiments.

Another hypothesis that will be proven is that despite the

meters, with no plastic strain or plastic strain path dependence.

dependent and the gradient plasticity, $31$ gradients, i.e. conditions that require utilization of scale-

history-independent surface of the perfect plasticity (Fig. 13). This

arguments in favor of the postulate of the perfect plasticity have

that (2) strain-induced anisotropy and path dependence do not

statement means that (1) the strain hardening is saturated, and

values

known that the yield surface in the six-dimensional space of

pressure and sample thickness distributions.

fourth-order elastic constants of diamond, which are not well

pressure are available. We assume $\mu = \mu_0 + C\sigma$, with two material parameters.

In addition, some of the third-order elastic constants of W and

fourth-order elastic constants of diamond, which are not well

defined from the literature, are refined by comparison with DAC

pressure and sample thickness distributions.

To summarize, in comparison with ref. $27$, current model

includes fourth-order elasticity of diamond, combined Coulomb

and plastic contact sliding, and linear pressure dependence of the

Coulomb friction coefficient. Moreover, all unknown material

parameters are calibrated using one set of experimental data and

verified using another experimental set.

Results

All four material parameters in the pressure dependence of the

yield strength and friction coefficient were calibrated by minimizing

the error between experimental and FEM results for pressure distributions for two curves with maximum pressures $p_{\text{max}} = 170$ and $240$ GPa (Fig. 2a). This led to

\[ \sigma_y = 1.8 + 0.1 p; \quad p \leq 225 \text{ GPa}; \quad \mu = 0.05 + 0.001 \sigma; \quad \sigma_c \leq 37 \text{ GPa}. \] (1)

Unexpected strong limitations on pressure and contact stress

appear because we found in FEM solutions that Coulomb sliding

and plastic flow do not occur for $\sigma_c > 37$ GPa and $p > 225$ GPa, respectively. With properties in Eq. (1), good correspondence is obtained for two other pressure distributions with $p_{\text{max}} = 300$ and $400$ GPa, with a maximum difference not exceeding 10% (Fig. 2a).

In addition, the profile of the sample after very large compression

and deformed anvil surface were reproduced for all four pressures,

with a maximum discrepancy smaller than $1 \mu$m (Fig. 2b, c). Both
discrepancies are within error for an experiment under such extreme conditions. As seen in Fig. 2, properties in Eq. (1) result in having good agreement with experimental pressure distribution not only at large pressures, but also at low pressures where the error in the experimental results is assumed to be the least. The achieved good agreement at lower pressures is missing in ref. $27$. Besides, thickness profiles are properly reproduced. The curves in Fig. 2 are nontrivial, and coincidence demonstrates strong verification of the entire model and the specific material properties from Eq. (1). It also proves the validity of the postulate of the perfect plasticity for W, which was directly incorporated in our model, and sufficiency of the local elastoplastic model even at micron scale and with huge stress and plastic strain gradients. In summary, elastoplasticity and, consequently, plastic friction under such large strain and pressure is plastic strain-, plastic strain path-, and scale-independent, which drastically simplifies theory and measurements.

In addition, the higher-order elastic constants of W and diamond, which have large scatter in literature (see the Methods section), have been also refined/identified. Thus, we found the third-order constants for W, $m = -1081$ and $n = -1164$ GPa, to obtain a slightly better fit to the experimental pressure distribution curves for three lowest pressure. The fourth-order elastic constant of diamond, $C_{1112} = 31,214$, $C_{1122} = 20,044$, and $C_{1266} = 819$ GPa, were found from the best fit to the sample profile under highest pressure only under constraint that they satisfy the known equation of state of diamond; see the Methods section.

The suggested method has high throughput features, which allows to determine ten material parameters using three pressure and one sample thickness distributions.

Known $^5$ pressure dependence of the yield strength for W has huge scatter (Fig. 3), which is related to numerous assumptions for the determination of $\sigma_y(p)$ and to attribution of the dependence of $\sigma_y$ on plastic strain to the pressure dependency. In our curve, the effect of plastic strain is excluded and the correctness of Eq. (1) is confirmed by numerous data in Fig. 2.
After proving its validity, the model is used for computational reconstruction of all fields of interest. Distribution of shear friction stress and normalized radial sample velocity along the diamond-sample contact surface at different pressures is shown in Fig.4a, b. Such a complex profile of shear stresses and their evolution are nontrivial and counterintuitive. In particular, shear stress in the sticking zone makes several oscillations in a central cup region, and the sticking zone grows with increasing compression. The plastic friction zone is surprisingly narrow, which does not allow use of the traditional method for determination of τ_y(p), based on a pressure gradient. The maximum yield strength in shear and corresponding p in the plastic sliding zone reduces from 5.85 GPa and 77.2 GPa for p_{max} = 164 GPa to 3.7 GPa and 44 GPa for p_{max} = 380 GPa. The maximum shear stress in the Coulomb sliding zone is 3.21 GPa, corresponding to σ_c = 37 GPa; for p_{max} = 380 GPa, it is 2 GPa, corresponding to σ_c = 26.2 GPa. An important conclusion is that, due to significant increase in the sticking zone, an increase in p_{max} does not lead to an increase in the maximum range of σ_c and friction stress, either for Coulomb or plastic friction. The only way to increase these ranges is to use torsion under a fixed force in rotational DAC for which FEM simulations show that the sticking zone is localized near the center.

The sample particles' radial velocity along the diamond-sample contact surface (Fig. 4b) is directed toward the center in the sticking zone for any pressure, and is equal, by the definition of sticking, to the velocity of the diamond contact particles. Outside the sticking zone, sample particles move away from the center, achieving maximum velocity at the edge of the culet. The maximum velocity increases to p_{max} = 231 GPa, then reduces due to the increasing sticking zone.

All relevant fields in the central part of the W sample at maximum pressure of 300 GPa are presented in Fig. 5 on a quarter of the sample, due to the symmetries. While axial stress σ_{zz} is independent of the z coordinate, radial stress σ_{rr} visibly depends on z and pressure p, by definition, in between.

All components of plastic strain and q are very heterogeneous and reach very large values. Plastic shear strain ε_{rz}^p (defined in Eq. (6)) changes sign three times in the central zone. Accumulated plastic strain q reaches its maximum value at the contact surface, especially where the thickness is smallest. Note that, for uniaxial compression/tension, q reduces to the logarithmic strain, and maximum q = 5.77 in Fig. 5c corresponds to the ratio of the initial-to-final length of exp(5.77) = 321. With increasing radius, q increases further. Material rotation in Fig. 5c, which leads to the development of texture, is also very large, with a maximum of 46.8° in this region. Thus, if strain-induced anisotropy would be...
present, isotropic flow theory would not describe experiments. The rotation angle, similar to shear stress $\sigma_{rz}$, is zero at the symmetry axis and plane and increases with increasing $r$ and $z$. Radial velocity (Fig. 5d) at such a pressure is directed toward the center in the entire region. It is independent of $z$ and its magnitude increases with $r$. The rate of accumulated plastic strain $q$ also increases with $r$, with zero region to the left of the white line in Fig. 5d, where plastic flow stops and the material deforms elastically. Evolution of the elastic zone with increasing pressure is shown in Fig. 2a. It appears at $p_{\text{max}} = 200$ GPa and increases with increasing pressure due to cupping of diamond.

Similar fields for three other maximum pressures, which we used for calibration and verification of the model, are given in Figs 6–8. For lower pressures, we present components of the stress tensor and pressure only in Fig. 9.

In the maximum pressure range from 170 to 380 GPa, axial stress $\sigma_{zz}$ is independent of the $z$ coordinate, radial stress $\sigma_{rr}$ shows visible dependence on $z$ and pressure $p$ is in between. Degree of heterogeneity of $\sigma_{rr}$ and $p$ increases with reducing maximum pressure because of more intense plastic flow. With further maximum pressure reduction, $\sigma_{zz}$ acquires some heterogeneity at the center of the sample and around corner point between beveled and initially flat central part. The heterogeneity of $\sigma_{zz}$ is quite pronounced in the entire central region for maximum pressure in the range of 1 to 10 GPa, while below the beveled part of the anvil $\sigma_{zz}$ and even pressure is quite homogeneous along $z$ coordinate. Shear stresses have generally similar patterns for any maximum pressure, governed by zero stress at the symmetry plane and axis and increasing shear stress with increasing $z$ and $r$. In the pressure range from 1 to 10 GPa, maximum shear stress is smaller than the yield strength in shear and either sticking or Coulomb friction are involved. Due to increase in the yield strength, maximum shear stress increases when maximum pressure growth from 10 to 100 GPa, then it reduces due to the
effect of significant cupping. Some cupping is first visible at $p_{\text{max}} = 170$ GPa and is quite pronounced at $p_{\text{max}} = 380$ GPa. However, region with elastic deformations without plasticity at the center of the sample is getting visible at $p_{\text{max}} = 240$ GPa and increases with further loading.

All stress fields in the central part of the diamond for $p_{\text{max}} = 300$ GPa are presented in Fig. 10. All normal stresses have their maximum at the center of the culet, with $\sigma_{\text{max}}^{zz} = -321$ GPa and $\sigma_{\text{max}}^{rr} = \sigma_{\text{max}}^{\theta\theta} = -260$ GPa, i.e. nonhydrostaticity is very high. Maximum shear stress $\sigma_{\text{max}}^{rz}$ is located away from the culet. This value is significantly smaller than the theoretical shear strength of 96.6 GPa at zero pressure, which grows with pressure. It is important that the regions in which maximum normal and shear stresses occur do not overlap.

The obtained fields of all components of the stress tensor are the basis for the development of criteria for fracture of diamond. To illustrate the concept, consider experimentally observed fracture due to compression stress $\sigma_{[110]}$ along the [110] direction. Theoretical strength for compression along the [110] direction obtained in refs.38,39 using ab initio simulations can be approximated as $\sigma_{[110]}^{\text{th}} = -471 + 1.64\sigma_{[110]}^G$ GPa, where $\sigma_{[110]}^G$ is the averaged biaxial normal stress in planes orthogonal to (110); in our case $\sigma_{[110]}^G = 0.5(\sigma_{[110]}^{[110]} + \sigma_{[00]}^{[110]})$, where $\sigma_{[110]}^{[110]}$ is normal stress along the [110]. The equivalent normalized stress in direction [110], plotted in Fig. 10, is then $\sigma_{[110]}^{[110]} = \sigma_{[110]}^{[110]} / \sigma_{[110]}^{\text{th}}$, and fracture occurs at...
and veriﬁcation of elastoplastic behavior under very large strains and pressures: order elastic constants, we justify some general unique properties of the yield strength and friction, as well as higher-order components of stress and large plastic strain tensors in W and DAC under extreme pressure. In particular, we re-introduce defects into simulations will open the possibility of providing the upper bound of achievable pressure (stresses), which will allow optimization of the design of anvils and loading conditions for a perfect crystal, as well as all complex tensorial information about elastoplastic properties and friction rules, as well as the development of criteria for fracture of diamond.

In summary, we suggested a novel coupled experimental—theoretical—computational approach that allowed us (using known experimental data from ref. 9) to extract complete information about elastoplastic properties and friction rules, as well as all complex tensorial fields for materials compressed in a DAC under extreme pressure. In particular, we reﬁned, calibrated, and veriﬁed models for elastoplastic behavior of a sample and contact friction for W up to 400 GPa and reconstruct ﬁelds of all components of stress and large plastic strain tensors in W and diamond. In addition to quantitative information on the pressure dependence of the yield strength and friction, as well as higher-order elastic constants, we justify some general unique properties of elastoplastic behavior under very large strains and pressures:

(a) Despite the generally accepted strain-induced anisotropy, strain hardening, and path-dependent plasticity, W after plastic deformation in diamond does not occur.

(b) Despite the µ-sized sample thickness and huge stress (5 GPa/µm) and plastic strain gradients, scale-independence of elastoplastic properties is found.

Both of these properties drastically simplify plasticity theory and measurements under extreme conditions.

Our ﬁnding for plasticity also implies important properties for plastic friction under such extreme loading: Plastic friction is plastic strain-, plastic strain path-, and scale-independent.

The developed experimental—theoretical—computational approach allows different realizations for different available experimental data. In particular, recently developed nanoscale sensing platform,40 which integrates nitrogen-vacancy color centers directly into the culet of diamond anvils, allows experimental determination of distribution of all six components of the stress tensor in diamond along the flat culet, i.e., at the contact surface with the sample. This information allowed us to reconstruct nontrivial normal and shear contact stresses between diamond and gasket and ﬁelds of all components of stress tensor in the entire anvil.

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Note that W is used as a gasket material in DAC at megabar pressures, i.e. obtained results have also applied importance for study of various sample materials within W gasket. Knowledge of the distributions of all (generally 12) components of stress and plastic strain tensors in a sample will allow study of their (instead of pressure alone) effect on phase transformations, chemical reactions, and various physical properties. In comparison with research under hydrostatic pressure, this will add up to 11 new dimensions to the parametric space for studying these processes, searching for new phases and materials, drastically reducing the required pressure for synthesis of new and known materials with unique properties, and understanding processes in the deep interiors of the Earth and other planets. Obtained results will also enable calibration and verification of known and new methods for measurement of the components of stress tensors in anvils and samples.

METHODS

A complete system of equations for fourth-order elasticity of diamond, large elastoplastic deformation of W, and combined Coulomb and plastic...
Geometry and boundary conditions

Axisymmetric problem formulation is considered. Due to symmetry of the Mao-type DACs used in ref. 27, only the upper part of the DAC and sample will be used in simulations. Geometry of the sample and the anvil, as well as the boundary conditions, are shown in Fig. 11 and are as follows:

(1) A uniform vertical displacement is applied at the boundary between the top inclined surface of the anvil and Boehler-type seat (line CD).

(2) At the symmetry axis \( r = 0 \) (line AB), shear stress \( \tau_{rz} \) and horizontal displacements are zero. At the symmetry plane \( z = 0 \), shear stress \( \tau_{rz} \) and vertical displacement are zero.

(3) At the contact surface between the gasket and the anvil, a combined Coulomb friction and plastic friction model, which is described below, is utilized.

(4) Other surfaces not mentioned above are stress-free.

Finite element algorithms for solution of the boundary-value problems are presented in Feng et al. 28

Friction model

According to the combined Coulomb friction and plastic friction model, there is complete cohesion between the contact pairs unless the shear (friction) stress reaches the critical value:

\[
\tau_{\text{crit}} = \min \left[ \mu \sigma_c, \tau_y(p) \right].
\]

(2)

When friction stress reaches \( \tau_{\text{crit}} \), contact sliding occurs in the radial direction. The critical shear stress \( \tau_{\text{crit}} = \mu \sigma_c \) is related to the Coulomb friction, where \( \mu \) is the friction coefficient and \( \sigma_c \) is the normal contact stress. However, the Coulomb friction stress cannot exceed the yield strength in shear \( \tau_y(p) \), which is defined in terms of the yield strength under compression, \( \sigma_y \), by \( \tau_y = \sigma_y / \sqrt{3} \), based on the von Mises yield criterion. Thus, plastic sliding occurs when the Coulomb friction exceeds \( \tau_y(p) \). In fact, it represents plastic shear flow within a very thin material layer immediately below the contact surface.

In this study the yield strength and the friction coefficient are assumed to be pressure and contact pressure dependent, respectively.

We assume \( \mu = 0.05 + 0.001 \sigma_c \), with two material parameters, which after calibration, looks like

\[
\mu = 0.05 + 0.001 \sigma_c, \quad \sigma_c \leq 37 \text{ GPa}.
\]

(3)

Limitations on the contact stress exist because in FEM solutions, Coulomb sliding does not occur for \( \sigma_c > 37 \text{ GPa} \), even for the highest maximum pressure of 380 GPa.

Elastoplastic material model under large strains and high pressure

We designate single and double contractions of the second-order tensors \( A = \{A_{ij}\} \) and \( B = \{B_{ij}\} \) over one and two indices as \( A : B = \{A_{ij}B_{ji}\} \) and \( A : B = \{A_{ij}B_{ji}\} \), respectively. The subscript ‘e’ denotes symmetrization, and the subscripts ‘r’ and ‘p’ denote elastic and plastic part of a tensor, respectively. The superscripts -1 and ‘T’ designate the inverse and transposition of a tensor. \( I \) is the second-order unit tensor.

The complete system of equations for a large elastoplastic deformation of a sample is as follows:\n
\[
\text{Decomposition of the deformation gradient } F \text{ in to elastic } F_e \text{ and plastic } F_p \text{ parts}
\]

\[
F = \partial r / \partial \bar{r} = F_e \cdot F_p = V_e \cdot V_p = V_e \cdot V_p \cdot R_e.
\]

(4)

where \( r \) and \( \bar{r} \) are the position vectors of material points in the actual (deformed) configuration and the reference (undeformed) configuration, respectively; \( V_e \) and \( V_p \) are symmetric elastic and plastic left stretch tensors, respectively, \( U_p \) is the plastic right stretch tensor, and \( R_e \) is the proper orthogonal elastic rotation tensor.

Elastic strain \( B_e \) and its Jaumann objective time derivative

\[
B_e = 0.5( F_e \cdot F_e^T - I), \quad \dot{B}_e = B_e - 2( W \cdot B_e ).
\]

(5)
Plastic strain (plotted in Figs 5–8)

$$\varepsilon_p = \frac{1}{2} \mathbf{R} \cdot (\mathbf{U}_p - \mathbf{U}_0 - \mathbf{I}) \cdot \mathbf{R}^T,$$

(6)

Decomposition of the velocity gradient I, into symmetric deformation rate d and skew symmetric spin w

$$\mathbf{I} = \mathbf{w} + \mathbf{d} \rightarrow \mathbf{d} = \mathbf{B}_s - 2(\mathbf{d} \cdot \mathbf{B}_s)_1 + \mathbf{V}_s \cdot \mathbf{D}_p \cdot \mathbf{V}_s, \quad \mathbf{D}_p = \mathbf{R}_a \cdot (\mathbf{U}_p - \mathbf{U}_p^{-1}) \cdot \mathbf{R}_a^T,$$

(7)

where $D_p$ is the plastic deformation rate.

Isotropic elasticity rule

$$\sigma = J^{-1}(2\mathbf{B}_s + \mathbf{I}) \frac{\partial \Psi}{\partial \mathbf{B}_s},$$

(8)

Here $\sigma$ is the true Cauchy stress, $J = \det \mathbf{F}$ is the Jacobian, and $\Psi$ is the specific Helmholtz free energy per unit undeformed volume.

Pressure-dependent yield surface (surface of perfect plasticity)

$$\varphi = \sqrt{(3/2)s : \mathbf{s} - \sigma_y(p) = 0},$$

(9)

where $s$ is the deviatoric part of Cauchy stress $\sigma$, and $\sigma_y$ is the yield strength in compression.

Plastic flow rule

$$\mathbf{D}_p = \lambda / \sqrt{\varphi} \mathbf{s} \cdot \mathbf{s},$$

(10)

where $\lambda \geq 0$ is a scalar determined from the consistency condition $\varphi = 0$.

The rate of accumulated plastic strain (plotted in Figs 5–8)

$$\dot{q} = (2\mathbf{D}_p : \mathbf{D}_p) / 3^{0.5} = \sqrt{2/3\lambda}.$$

(11)

Equilibrium condition

$$\nabla \cdot \mathbf{\sigma} = 0,$$

(12)

where $\nabla$ is the divergence operator in the deformed configuration.

The yield strength in compression

We assume $\sigma_y = c_0 p + \sigma_y$ with two material parameters, which, after calibration, results in

$$\sigma_y = 1.8 + 0.1p; \quad p \leq 225 \text{ GPa}.$$ (13)

Limitation on the pressure exists because, in FEM solutions, plastic flow does not occur for $p > 225$ GPa, despite the maximum pressure of 380 GPa.

Nonlinear isotropic elasticity for sample

The third-order nonlinear elastic Murnaghan potential is utilized:

$$\Psi(B_s) = \frac{\lambda + 2G}{2} (I - 2GL) + I + \frac{2m}{3} (n - 2ml) I,$$

(14)

where $\lambda$, $G$, $I$, $m$, $n$ are material parameters and $I$, $I$, $I$ are invariants of the elastic strain tensor:

$$I_1 = \text{trace} (B_s), \quad I_2 = B_{22}B_{33}B_{11} - B_{12}B_{12}B_{12} - B_{13}B_{13}B_{13} - B_{23}B_{23}B_{23}, \quad I_3 = \det B_s.$$ (15)

Furthermore, we have:

$$\frac{\partial \Psi}{\partial \mathbf{B}_s} = I, \quad \frac{\partial \Psi}{\partial \mathbf{B}_s} = -B_s + \mathbf{I}.$$

(16)

Therefore, according to the elasticity rule Eq. (8), the Cauchy stress can be determined as:

$$\sigma = J^{-1}(2\mathbf{B}_s + \mathbf{I}) \left[ \lambda I + 2G \mathbf{B}_s + B_{11}I + 2m I - 2ml \mathbf{B}_s - 2mn \frac{\partial \Psi}{\partial \mathbf{B}_s} \right].$$

(17)

Nonlinear anisotropic elasticity for diamond

To study the finite elastic strains in diamond, a free energy which includes the fourth-order terms of the Lagrangian strains $E_0 = 0.5(F_0^2F_0 - \mathbf{I})$ is utilized as

$$\Psi = \frac{1}{2} C_{111} (n_1^3 + n_2^3 + n_3^3) + C_{112} (n_1 n_2 + n_1 n_3 + n_2 n_3) + \frac{1}{3} C_{114} (n_1^2 + n_2^2 + n_3^2) + \frac{1}{4} C_{115} (n_1 + n_2 + n_3) + \frac{1}{2} C_{116} (n_1 n_2 + n_1 n_3 + n_2 n_3) + \frac{1}{6} C_{117} (n_1^2 + n_2^2 + n_3^2),$$

(18)

where

$$n_1 = E_{x11}, \quad n_2 = E_{x22}, \quad n_3 = E_{x33}, \quad n_4 = 2E_{x33}, \quad n_5 = 2E_{x31}, \quad n_6 = 2E_{x32}.$$ (19)

Therefore, based on the elasticity law, the Cauchy stress in the diamond can be determined as:

$$\sigma = J^{-1}(2\mathbf{B}_s + \mathbf{I}) \frac{\partial \Psi}{\partial \mathbf{B}_s}.$$ (20)

Material properties

Diamond. All elastic material constants are taken from Telichko et al., which, to the authors’ knowledge, is the only reference that provides all third- and fourth-order elastic constants for diamond. These were determined using first principle simulations. Thus, we used the following elastic constants in our simulations:

$$C_{11} = 1081.9 \text{ GPa}, \quad C_{22} = 125.2 \text{ GPa}, \quad C_{44} = 578.6 \text{ GPa},$$

(21)

$$C_{111} = -7611.1637 \text{ GPa}, \quad C_{112} = -640 \text{ GPa}, \quad C_{114} = -400 \text{ GPa}, \quad C_{115} = -1148 \text{ GPa},$$

(21)

$$C_{116} = 26.687 \text{ GPa}, \quad C_{117} = 31.214 \text{ GPa}, \quad C_{122} = 20.044 \text{ GPa}, \quad C_{132} = -425 \text{ GPa}, \quad C_{133} = -1385 \text{ GPa}, \quad C_{222} = -264 \text{ GPa},$$

(21)

$$C_{233} = -819 \text{ GPa}, \quad C_{333} = -487 \text{ GPa}, \quad C_{444} = -11 \text{ GPa}, \quad C_{466} = 528 \text{ GPa}.$$ (21)

Since available data for the third-order elastic constants from different references have significant scatter, we assume that some of the fourth-order elastic constants are not precise either. Indeed, for the elastic constants from Telichko et al., we were unable to obtain the experimental equation of state collected in Maezono et al. Thus, we changed $C_{1112}$, $C_{1222}$, and $C_{2266}$ to the values indicated in Eq. (21) in order to receive good correspondence with the equation of state from Sato et al.; see Fig. 12, and sample profile at highest pressure, see Fig. 2c.

A majority of equations of state of diamond determined by different methods falls in between those from Sato et al. and McSkimin and Andreatch. Modifying the higher-order elastic properties of the diamond is another advancement over ref. 27.
The elastic constants of the polycrystalline tungsten from Vekilov et al. are used in this study, with some modifications:

$$\lambda = 206.5, \quad G = 150.3, \quad l = -404, \quad m = -1, \quad n = -1164 \text{ GPa}. \quad (22)$$

The third-order constants $m$ and $n$ for polycrystal have been found from the elastic constants for single crystal using the simplest Voight averaging scheme. Thus, they may have significant indeterminacy. We changed $n$ and $m$ to obtain a slightly better fit to the experimental pressure distribution curves for three lowest pressures.

Geometric interpretation of the postulate of perfect plasticity is presented in and Fig. 13.

**DATA AVAILABILITY**

The authors declare that the main data supporting the findings of this study are available within the article. Extra data are available from the corresponding author upon request.

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AUTHOR CONTRIBUTIONS

V.I.L. designed and supervised research, developed model, analyzed results and wrote paper. M.K. modified and extended the FEM algorithm, performed all simulations, and participated in analysis and writing paper. B.F. developed FEM algorithm and ABAQUS subroutines.

COMPETING INTERESTS

The authors declare no competing interests.

ADDITIONAL INFORMATION

Correspondence and requests for materials should be addressed to V.I.L.

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