Supplementary file

Multi-scale evaluation of mechanical properties of granite under microwave irradiation

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1. Calculation of macro-mechanical parameters

In addition to easily measurable parameters such as peak strength and peak strain, other macro-mechanical parameters can be derived from the stress-strain curve characteristics to investigate the impact of microwave treatment on the mechanical properties of granite. The mid-body strain is calculated as follows (Brady and Brown, 2007):

$$\varepsilon_v = \varepsilon_1 + 2\varepsilon_3 \tag{1}$$

where ε_v represents the volumetric strain; ε_1 represents the axial strain; ε_3 represents the circumferential strain. In addition, the elastic modulus and Poisson's ratio of rocks can be calculated as follows (Brady and Brown, 2007):

$$E = \frac{\sigma_b - \sigma_a}{\varepsilon_b - \varepsilon_a} \tag{2}$$

$$\upsilon = \frac{\varepsilon_{dp}}{\varepsilon_{lp}} \tag{3}$$

where σ_a, σ_b represent the starting and ending stress values of the straight line segment in the stress-strain curve, respectively, MPa; ε_a, ε_b represent the starting and ending strain values of the straight line segment in the stress-strain curve, respectively; ε_{dp}, ε_{lp} represent the average values of the strain in the corresponding straight line segment portion on the stress-annular strain curve and stress-axial strain curve, respectively.

2. Calculation of micro-mechanical parameters

The Oliver-Pharr method is a commonly utilized international analytical technique for determining micro-mechanical parameters such as hardness and Young's modulus at the maximum indentation depth.

The contact stiffness is specified as the slope of the tangent line at the maximum load on the unloading curve, and it can be expressed as:

$$S = \left.\frac{dP}{dh}\right|_{h=h_m} \tag{4}$$

The reduced modulus is calculated as:

$$E_r = \frac{\sqrt{\pi}}{2\beta} \cdot \frac{S}{\sqrt{A_c}} \tag{5}$$

The contact area A_c is related to the contact depth h_c, which can be expressed as:

$$A_c = f\left(h_c\right) \tag{6}$$

For the Berkovich indenter, the contact depth can be expressed as:

$$h_c = h_m - \varepsilon \frac{P_m}{S} \tag{7}$$

Hardness is calculated as:

$$H = \frac{P_m}{A_c} \tag{8}$$

According to the Hertz contact theory (Hertz, 1881), the Young's modulus of a material can be calculated as follows:

$$E = \left(1 - v^2\right)\left[\frac{1}{E_r} - \frac{1 - v_i^2}{E_i}\right]^{-1} \tag{9}$$

where β represents the indenter correction factor and ε is a constant related to the shape of the indenter. For the Berkovich indenter, $\beta = 1.034$ and $\varepsilon = 0.75$. Among the parameters, h_c denotes the contact depth; A_c denotes the contact area that can be expressed as $A_c = 24.56h_c^2$ (Oliver and Pharr, 1992); E_r is the reduced modulus, which represents the interaction effect between the indenter and the material; E_i and v_i denote the Young's modulus and Poisson's ratio of the indenter, respectively. For the diamond indenter used in this study, E_i = 1141 GPa and v_i = 0.07. v is the Poisson's ratio of the indented material. This can be reasonably assumed based on the relevant literature (Mavko et al., 2020). The explanation is that a sensitivity analysis of the Poisson's ratio with 40% uncertainty shows that the uncertainty in Young's modulus is only 5% (Hay, 2009).

3. Micro-fracture toughness calculation

The authors chose the energy analysis method (Cheng et al., 2002) to calculate fracture toughness, which obtains this parameter simply on the basis of the single load-displacement curve of the nanoindentation. During nanoindentation, the total energy (U) is composed of two elements: elastic energy (U_e) and plastic energy (U_p). The plastic energy (U_p) in turn consists of two elements: induced fracture energy (U_{frac}) and pure plastic energy (U_{pp}). The specific energy balance equation is expressed as follows (Cheng et al., 2002; Ma et al., 2020):

$$U = U_e + U_p = U_e + U_{pp} + U_{frac} \tag{10}$$

where U and U_e can be gained by integrating the loading and unloading curves over the load-displacement curve.

According to the linear elastic fracture mechanics, the fracture toughness K_{IC} can be calculated for plane strain conditions (described below):

$$K_{IC} = \sqrt{G_c E_r \left(1 - v^2\right)} \tag{11}$$

This equation applies to thick boards, such as rocks and minerals, where the constraining effect of deformation in the thickness direction results in no strain in the z direction, i.e., $\varepsilon_z = 0$. This state, where strain exists in only two directions, is called the plane strain case. Here, E_r represents the reduced modulus and G_c represents the strain energy release rate. Gc can be calculated by:

$$G_c = \frac{\partial U_{frac}}{\partial A_c} = \frac{U_{frac}}{A_c} \tag{12}$$

where A_c represents the projection contact area and U_{frac} can be calculated from Equation (10), expressed as:

$$U_{frac} = U_p - U_{pp} = U - U_e - U_{pp} \tag{13}$$

Although U and U_e are known, U_{pp} cannot be directly determined from curves but it is typically obtained through a combination of experimental and finite element simulation results. According to Cheng et al. (2002), U_{pp} can be expressed as:

$$U_{pp} = \left\{ 1 - \left[\frac{1 - 3\left(\frac{h_f}{h_{\max}}\right)^2 + 2\left(\frac{h_f}{h_{\max}}\right)^3}{1 - \left(\frac{h_f}{h_{\max}}\right)^2} \right] \right\} U \tag{14}$$

The fracture toughness can be obtained by substituting it into Equation (13), (12), and (11) sequentially. In this process, it is not necessary to measure the length of the crack.

4. Upscaling calculation

(1) Self-Consistent method

On the basis of the equilibrium of strain energy stored or dissipated by the material over a certain volume range, the Self-Consistent method (S-C method) replaces anisotropic composites with an idealized homogeneous continuum. The mechanical behavior of the two media is the same when the scale range is much larger than the local characteristic dimensions of the anisotropic material. The effective modulus of the composite material can be expressed as follows:

$$\bar{C} = C_0 + \sum_{r=1}^{N-1} c_r \left(C_r - C_0\right)\left[I + \bar{P}_r\left(C_r - \bar{C}\right)\right]^{-1} \tag{15}$$

where C_0 and C_r represent the modulus of the mineral with the largest content and the modulus of the rth phase mineral, respectively; c_r represents the volume fraction of phase r; I represents a tensor related to the inclusions' shape; $\bar{P}_r$ represents the P tensor when the phase r is placed in an unknown composite material used as a matrix. $\bar{P}_r$ is related to the shape of the inclusions and the modulus of the unknown composite $\bar{C}$. The above is the implicit equation for the effective modulus of the composite.

By using a simplified algorithm for the isotropic tensor, implicit equations for the effective shear modulus and bulk modulus of granite were obtained (Lei et al., 2021b):

$$\begin{cases} G^{hom} = \sum_{r=0} c_r \dfrac{5G_r \cdot G^{hom}\left(3K^{hom} + 4G^{hom}\right)}{G^{hom}\left(9K^{hom} + 8G^{hom}\right) + 6G_r\left(K^{hom} + 2G^{hom}\right)} \\ K^{hom} = \sum_{r=0} c_r \dfrac{K_r\left(3K^{hom} + 4G^{hom}\right)}{3K_r + 4G^{hom}} \end{cases} \tag{16}$$

where G^{hom} and K^{hom} denote the effective shear modulus and bulk modulus of the homogenized granite, respectively; G_r and K_r are the shear modulus and bulk modulus of phase r, respectively. The calculation equation is as follows:

$$\begin{cases} G_r = \dfrac{E}{2(1+v)} \\ K_r = \dfrac{E}{3(1-2v)} \end{cases} \tag{17}$$

(2) Voigt-Reuss-Hill method

The Voigt-Reuss-Hill method (V-R-H method) takes into account the link between the elastic behavior of aggregates and single crystals. Therein, the Voigt boundaries (upper boundaries) and Reuss boundaries (lower boundaries) are the average elastic properties of multiphase and polycrystalline aggregates, respectively (Hill, 1952). The average values provide a convenient way of estimating the rock properties of aggregates, without considering the orientation and interlocking of the particles.

The upper bound of the equivalent modulus for the n components is derived from the Voigt model (Voigt, 1928):

$$M_{\mathrm{V}} = \sum_{i=1}^{n} \varphi_i M_i \tag{18}$$

where φ_i and M_i represent the volume content and Young's modulus of the ith component, respectively. The Voigt model assumes that the components are isotropic and linearly elastic.

The lower bound of the equivalent modulus for the n components is derived from the Reuss model (Reuss, 1929):

$$\frac{1}{M_{\mathrm{R}}} = \sum_{i=1}^{n} \frac{\varphi_i}{M_i} \tag{19}$$

The Hill model (Hill, 1952) uses the average of the upper and lower boundaries to calculate the equivalent modulus:

$$M = \frac{1}{2}\left(M_{\mathrm{V}} + M_{\mathrm{R}}\right) \tag{20}$$

(3) Mori-Tanaka method

The Mori-Tanaka method (M-T method), proposed by Mori and Tanaka in 1973 (Mori and Tanaka, 1973), takes into account the interactions between inclusions and assumes that each inclusion is embedded in an infinitely large matrix. The homogenization process of the method is shown in Fig. 1. The effective modulus of the composite material can be expressed as follows:

$$\bar{C} = C_0 + \sum_{r=1}^{N-1} c_r \left[\left(C_r - C_0\right)^{-1} + c_0 P_r\right]^{-1} \tag{21}$$

The bulk and shear modulus of granite are expressed as follows:

$$\begin{cases} G^{hom} = \dfrac{\displaystyle\sum_{r=0} \frac{c_r G_r}{G_0\left(9K_0 + 8G_0\right) + 6G_r\left(K_0 + 2G_0\right)}}{\displaystyle\sum_{r=0} \frac{c_r}{G_0\left(9K_0 + 8G_0\right) + 6G_r\left(K_0 + 2G_0\right)}} \\ K^{hom} = \dfrac{\displaystyle\sum_{r=0} \frac{c_r K_r}{3K_r + 4G_0}}{\displaystyle\sum_{r=0} \frac{c_r}{3K_r + 4G_0}} \end{cases} \tag{22}$$

where K_0 and G_0 denote the bulk and shear modulus of Bit, respectively. Considering the obvious pore structure of Bit, the bulk modulus and shear modulus of Bit are expressed as follows:

$$\begin{cases} G_0 = \dfrac{\left(1-\varphi\right)G_s}{1 + 6\varphi \dfrac{K_s + 2G_s}{9K_s + 8G_s}} \\ K_0 = \dfrac{4\left(1-\varphi\right)K_s G_s}{4G_s + 3\varphi K_s} \end{cases} \tag{23}$$

where K_s and G_s represent the bulk modulus and shear modulus of Bit, respectively, independent of the pore structure; φ is the porosity of Bit. Considering the special laminar structure of Bit, this study set the percentage of pore volume in Bit to the total volume to 30%.

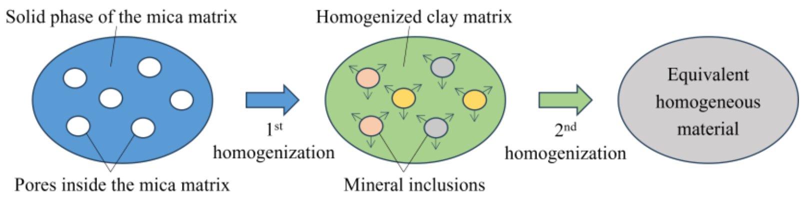

Fig. 1 Homogenization process of the M-T method

(4) Generalized Means method

The Generalized Means method (G-M method) is a semi-empirical model for predicting the mechanical properties of multiphase materials and polycrystalline rocks (Ji et al., 2004). The mechanical properties of multiphase materials in the G-M method are related to the volume fraction and composition of the material, which can be determined by the following equation (Ayatollahi et al., 2020; Ji et al., 2004):

$$M_{\mathrm{d}}(J) = \left[\sum_{i=1}^{n} \left(f_i M_i^{J} \right) \right]^{1/J} \tag{24}$$

$$\sum_{i=1}^{n} f_i = 1 \tag{25}$$

where the subscripts i and d stand for the ith phase and the multiphase material consisting of n phases, respectively; f_i denotes the volume fraction of each phase; M is a certain mechanical property; and J is the mesostructure coefficient, whose value depends on the mesostructure.

Note that the value of J for each multiphase material must be measured separately by multiple tests. For polycrystalline rocks (e.g., granite), Ayatollahi et al. (2020) found that the predicted Young's modulus matches very well with the results of uniaxial compression tests when J is infinitesimal. On the other hand, the predicted Young's modulus values are almost constant when J is beyond the range of (-50,50). Therefore, the authors chose J = -50 as the J value for the predicted modulus.

For the equivalent mechanical parameters of the four types of mineral media obtained by using the S-C and M-T methods, on the basis of the theory of elastic mechanics, the Young's modulus of the rock at the centimeter scale can be calculated using Equation (26):

$$E^{hom} = \frac{9K^{hom} \cdot G^{hom}}{3K^{hom} + G^{hom}} \tag{26}$$