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Finite Deformation by Elasticity, Slip, and Twinning: Atomistic Considerations, Continuum Modeling, and Application to Ceramic Crystals

by John D. Clayton

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14. ABSTRACT
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FINITE DEFORMATION BY ELASTICITY, SLIP, AND TWINNING: ATOMISTIC CONSIDERATIONS, CONTINUUM MODELING, AND APPLICATION TO CERAMIC CRYSTALS

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ABSTRACT: A continuum theory is developed for modeling elasticity, plasticity, and twinning in single crystals of arbitrary anisotropy, subjected to arbitrarily large deformations. Concepts from discrete lattice models are considered for estimating resistances to inelastic shear. Nonlinear thermoelastic calculations are used in conjunction with experimental shock physics observations to provide estimates for resistances to slip, twinning, and shear fracture on preferred planes in alumina single crystals (i.e., rhomobohedral corundum or sapphire).

INTRODUCTION: Large deformation theory is needed for an accurate description of finite shear strains associated with slip and deformation twinning and improper lattice rotations across twin boundaries. Nonlinear anisotropic elasticity is also necessary for accurately describing the response of ceramic single crystals to high pressure loading, for example plate impact or explosively driven shock (Graham & Brooks [1971]).

PROCEDURES, RESULTS, AND DISCUSSION: The deformation gradient $\mathbf{F}$ is decomposed multiplicatively as

$$F^{a}_{.A} = F^{Ea}_{.\alpha} F^{I\alpha}_{.\beta} F^{P\beta}_{.A} = F^{Ea}_{.\alpha} \bar{F}^{\alpha}_{.A}, \qquad (1)$$

where $\mathbf{F^E}$ accounts for thermoelasticity, $\mathbf{F^I}$ for twinning shears, and $\mathbf{F^P}$ for dislocation glide. Skew components of the covariant derivative of $\mathbf{F^P}$ can be used to construct a density of geometrically necessary dislocations associated with slip. In fact, Nye's [1953] theory followed from observations of slip traces in transparent corundum. A density of partial dislocations associated with incompatibility of twins follows from the gradient of $\mathbf{F^I}$. A net Burgers vector $\bar{\mathbf{b}}$ is, from integration over circuit C encircling reference area A with normal $\mathbf{N}$:

$$\bar{b}^{\alpha} = -\oint_C \bar{F}^{\alpha}_{.A} dX^{A} = \int_A \bar{\alpha}^{\alpha A} N_A dA, \qquad \bar{\alpha}^{\alpha A} = \varepsilon^{ABC} (\underbrace{F^{I\alpha}_{.\beta} F^{P\beta}_{.B,C}}_{\text{slip gradients}} + \underbrace{F^{I\alpha}_{.\beta,C} F^{P\beta}_{.B}}_{\text{twin partials}}). \qquad (2)$$

Contributions of slip gradients to the Burgers vector have been described elsewhere (Nye [1953], Clayton et al. [2005]). The final term on the right in the second of (2) results from gradients in twin fractions, e.g. interface dislocations at tapered twin boundaries. Disclination models of twins (Clayton et al. [2005]) could complement such a description. The Helmholtz free energy per unit relaxed volume of crystal is prescribed as

$$\bar{\Psi} = \underbrace{\frac{1}{2} E^E_{\alpha\beta} \bar{\mathbb{C}}^{\alpha\beta\chi\delta} E^E_{\chi\delta}}_{\text{second order elasticity}} + \underbrace{\frac{1}{6} E^E_{\alpha\beta} \bar{\mathbb{C}}^{\alpha\beta\chi\delta\varepsilon\phi} E^E_{\chi\delta} E^E_{\varepsilon\phi}}_{\text{third order elastic constants}} - \underbrace{\bar{\beta}^{\alpha\beta} E^E_{\alpha\beta} (\theta - \theta_0)}_{\text{thermoelastic coupling}} - \underbrace{\bar{c}\theta \log\left(\frac{\theta}{\theta_0}\right)}_{\text{specific heat}} + \underbrace{\bar{\Psi}^R}_{\substack{\text{lattice} \\ \text{defects}}} . \quad (3)$$

In (3), $\mathbf{E}^{\mathbf{E}}$ is the Green elastic strain, $\bar{\mathbb{C}}$ are elastic coefficients, $\bar{\boldsymbol{\beta}}$ are thermal stress coefficients, and $\bar{c}$ is the specific heat. Kinetic relations for slip and twinning are written

$$\dot{\gamma}^i = \dot{\gamma}_S \left| \frac{\bar{\tau}^i}{\bar{g}^i} \right|^m \frac{\bar{\tau}^i}{|\bar{\tau}^i|}, \qquad \dot{\gamma}^i_j = \dot{\gamma}_S \left| \frac{\bar{\tau}^i_j}{\bar{g}^i_j} \right|^m \frac{\bar{\tau}^i_j}{|\bar{\tau}^i_j|}, \qquad \dot{f}^j = \frac{\dot{\gamma}_T}{s^j} \left| \frac{\langle \bar{\tau}^j \rangle}{\bar{g}^j} \right|^p , \quad (4)$$

where $\dot{\gamma}^i$ and $\dot{\gamma}^i_j$ are slip rates for slip system *i* in the parent crystal and for slip system *i* in twin fraction *j*, $\dot{f}^j$ is the rate of evolving volume fraction of twin *j* with characteristic shear s^j, $\bar{\tau}$ is the resolved Eshelby or Kirchhoff stress, $\bar{g}$ are resistances that evolve with the thermodynamic state, and remaining terms are constants. The crystal structure and relevant systems for slip and twinning in sapphire are shown in Fig. 1. A full close-packed layer of O atoms lies in between each partially filled (0001) plane of Al atoms in the hexagonal cell.

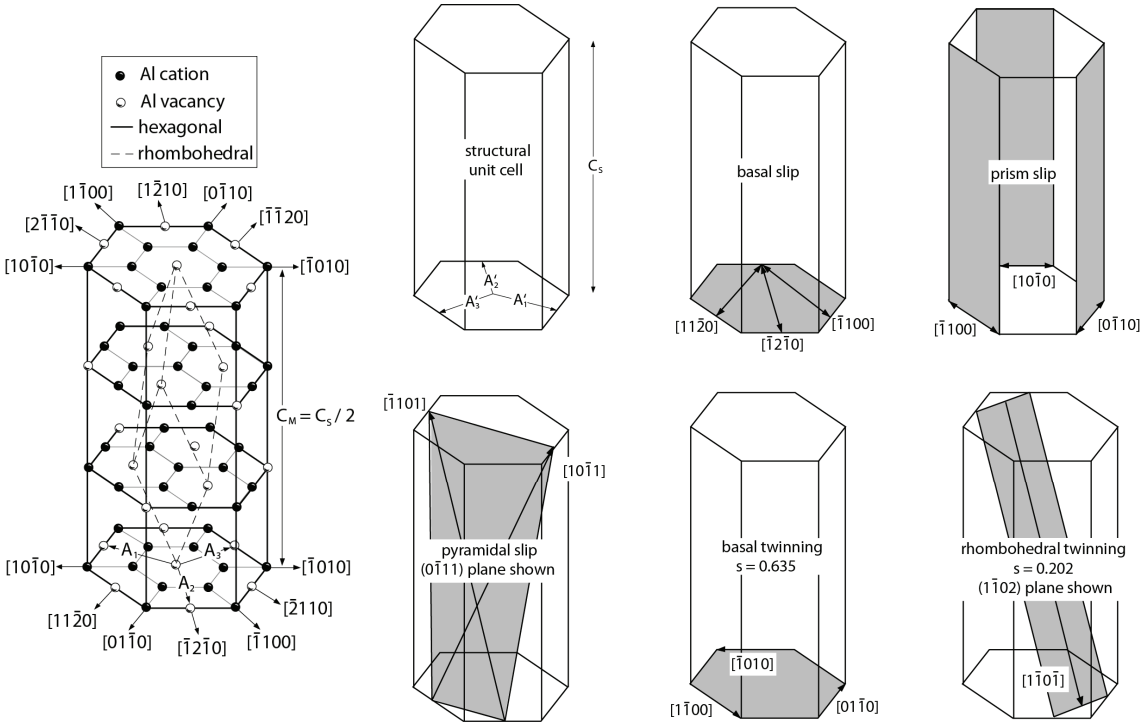

Fig. 1 Unit cells of sapphire, after Kronberg [1957], and slip and twin systems.

Because of sapphire's brittle nature, values of $\bar{g}$ must be inferred from experiments where confining pressures are high, such as shock loading (Graham & Brooks [1971]), indentation (Tymiak & Gerberich [2007]), or must be extrapolated from high temperature data. Previous research indicates that the Peierls stress concept may provide insight into to the low

temperature slip resistance (Farber et al. [1993]); the ratio of stacking fault energy to Burgers vector may approximate the twin nucleation stress; and the theoretical shear fracture strength of the crystal may be approached in shock physics experiments (Graham & Brooks [1971]). Values of these theoretical quantities are found as

$$\tau_C^{Peierls} = \left(2\mu / K\right)\exp\left(-2\pi d / \left(Kb\right)\right), \quad \tau_C^{twin} = W_{SF} / b, \qquad \tau_C^{fracture} = \mu b / \left(2\pi d\right), \quad (5)$$

where μ is the rhombohedral shear modulus, *K* accounts for dislocation line geometry and anisotropy, *b* is the magnitude of the local Burgers vector, *d* is the interplanar spacing, and W_{SF} is the appropriate stacking fault energy. Anisotropic nonlinear elasticity is used here to compute more accurate estimates for τ_C, and hence $\bar{g}$ in the limit of rate independent inelasticity. Resolved shear stresses for basal and prismatic slip, basal and rhombohedral twinning, and fracture on pyramidal and rhombohedral planes are calculated during uniaxial straining of single crystals of various orientations. Stress values computed at the Hugoniot elastic limit (Graham & Brooks [1971]) provide the bounds in the first data column of Table 1. These bounds compare favorably with those from indentation (Tymiak & Gerberich [2007]), but differ substantially from order-of-magnitude estimates computed via (5).

Table 1: Bounds on low temperature shear strengths for slip, twinning, and fracture.

Mechanism	τ_C [GPa] present work	τ_C [GPa] theory [(1)]	τ_C [GPa] indentation [(2)]
basal slip	$2.7 < \tau_C < 5.0$	9.0	$4.8 < \tau_C < 23.7$
prism slip	$2.3 < \tau_C < 5.7$	0.3	$2.5 < \tau_C < 4.1$
pyramidal slip	--	0.7	7.0
basal twin	$\tau_C > 4.0$	7.3	$4.8 < \tau_C < 7.3$
rhombohedral twin	$1.0 < \tau_C < 8.1$	3.6	$1.0 < \tau_C < 7.3$
prism fracture	$\tau_C > 5.9$	40.5	--
pyramidal fracture	$\tau_C > 6.7$	30.6	--
rhombohedral fracture	$\tau_C > 7.9$	34.4	--

[(1)]Equation (5) [(2)]Tymiak & Gerberich [2007]

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