THE MURNAGHAN PARAMETERS

In the usual application of linear elasticity theory, the bulk modulus of a crystal is defined as [7]

$$B_1 = -V\cdot\frac{dp}{dV}\Bigg|_{\sigma_{ij}(S_{ijkl},\,\tilde{R})\,=\,\bar{\sigma}} = f_1(1/s_{\mu\nu}) \qquad (4)$$

where $s_{\mu\nu}$ are the single-crystal second-order elastic compliances in the usual matrix notation, σ_{ij} are the stress tensors, $\tilde{R}$ is the rotation matrix, and f_1 is a functional constant dependent upon the crystal symmetry. Note that B_1, a scalar, is some linear combination of the elements of the second-order elasticity tensor. The Murnaghan parameters are thus given by [see, for example, Ref. 5]

$$B_O = \{ B_1^T\}_{p=0} \qquad (5)$$

and

$$B_O' = \{(B_1^T)'\}_{p=0} \qquad (6)$$

where the prime refers to isothermal pressure derivative and the superscript T denotes the isothermal value.

It has been shown experimentally [8] that the bulk modulus of polycrystalline aggregates cannot be given by Eq. (4). In light of the Voigt-Reuss-Hill (VRH) approximation [6],