Pseudo-Liquid (Hugoniot) and Particle-in-Matrix Modeling in Geologic Materials.

R. A. Graham, The Tome Group, 608 Cenizo Blvd., Uvalde, Texas 78801. tomecenzo@aol.com

Introduction: Pressure-volume states in solids at elevated temperatures have been determined over the past fifty years with shock-compression loading and sample response measurements. The resulting equations-of-state materials models assume precise control of loading and sample geometry, thermodynamic equilibrium, and homogeneity. Such "Hugoniot" modeling is essentially pseudo-liquid in nature, as known or unknown characteristic solid behaviors are applied to observed liquid-like data and called "strength effects." Development of the field of high-pressure shock-compression science is one of the most outstanding accomplishments of the late 20th Century; it is largely responsible for our present high pressure knowledge of planetary and earth materials. 21st Century shock-compression science is directed toward developing models for quantification of local heterogeneities, a modeling challenge orders-of-magnitude more difficult. I have characterized the modern efforts as "stirring the pseudo-liquid" [1]. Quantification of PDF processes in quartz requires development of a "Particle-in-Matrix Model" that explicitly models local effects at the particle (quartz grain) level and continues stirring of the pseudo-fluid based on PDFs as indicators of local stresses.

Planar Deformation Features in Quartz: Some of the most persistent and thoughtful work in impact metamorphism has been carried out in quartz from impact craters and in laboratory experiments [2,3,4]. The work has moved from PDFs as general indicators of a pressure range to their use in semi-quantitative measures of shock pressure [5]. It is generally agreed that PDF orientations are along selected crystallographic directions and that their orientation with respect to the c-axis and their numbers are a unique result of shock compression. Further, as Robertson [6] has related based on his PDF studies of Bee Bluff samples "*It is apparent that a total comprehension of quartz planar feature development has not been achieved and that attention and that attention should be focussed on porous lithologies*." When fully developed, the particle-in-matrix model will accomplish that goal.

Shock-Compression Science in Quartz: The first shock work on quartz under precise laboratory conditions was begun in the Physical Research Department of Sandia Corporation (National Laboratories) in 1959. The work involved measuring the piezoelectric responses of x-cut quartz under precisely controlled explosive and impact loading [7,8,9]. The startling result obtained showed a state of zero piezoelectric polarization above the Hugoniot-elastic-limit; quartz was transformed to a bulk-state of zero shear-stress. This observation was verified by conventional shock response measurements by Wackerle [10] and Fowles [11]. Observations of optical emission showed linear features oriented at 36 and 26 degrees to the optical axis. Further impact work on impact showed similar linear optical planar features in quartz and in piezoelectric lithum niobate. Grady [12] developed a model of localized deformation along specific crystallographic directions with thermal energies resulting from release of the large shear strains (5 to 10% of shear modulus) under shock compression. In Grady's model temperatures are kept above melt temperature for 100 nsec or so. The present understanding is that we can expect loss of bulk shear stress in strong-solids of low- thermal conductivity. As shown in Davison and Graham [13] the model was tested over a range of materials and found to be characteristic of high-strength, low-conductivity solids. All available shock-compression work supports a model process of localized slip at critical shear stresses.

How Can We Model Local Effects in Quartz? : There is evidence from observations of quartz in impact craters that particle size, morphology and orientation significantly affect PDF formation. It is a relatively straight-forward task to identify the problem conceptually, but a long and detailed study is needed to quantify the processes. Figure 1 shows overall features of the particle-in-matrix conceptual model.

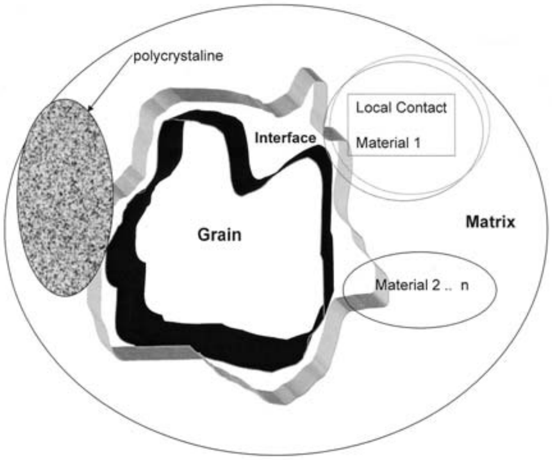

Figure 1. Typical particle-in-matrix modeling configurations to be quantified.

Note that starting from the grain level, each particle morphology is expected to strongly influence local deformation effects. Grains can be expected to have grain boundaries and internal structure. As deformation continues deformation interfaces will develop with local deformation depending upon the mechanical interaction between grain and matrix. In general the matrix may represent local contact or fully-contacting media. The local deformation can be easily shown to be in a shear-deformation space outside those available from macroscopic measurements. Thermal behaviors are directly dependent on the local deformations and thermal properties. Quantification and verification of a specific model requires a persistent, focused effort.

Current Status of Modeling: Over the past ten years significant progress has been made in developing the ability to calculate and quantify local processes in shock-compressed solids. PDF observations provide a defining basis for confirming theory as their presence provides the only capability available today to quantify grain-level effects. Describing the effects require shear stress prediction in the quartz particle. Most advanced modeling work is that of Horie [14,15], Baer [16] Eakins and Thadhani [17], and Dwivedi, et al [18]. Computer codes to incorporate characteristic local effects are in place in both 2-D and 3-D, but confirmation of calculations rests upon measurements at the macroscopic level. It is generally agreed that work is in an early development state.

Interesting Geologic Configurations: Two well-defined particle-matrix configuration are available from Bee Bluff target materials. The Carrizo Sandstone is essentially a highly porous compact of fine sandstone. The limonite present is of negligible strength. Its shock-transformed configuration is a well-bonded quartz compact resulting from melt at particle interactions. The quartz silt in the calcareous Indio siltstone consists of silt of random orientation in calcite particles.

Thus the sandstone is a porous quartz target with contacting local surfaces, a classical modeling problem. In contrast, isolated quartz grains in Bee Bluff Siltstone present a configuration of a hard grain of high strength in a soft, essentially hydrostatic medium, as calcite has low strength and deformed hydrostatically under shock deformation. The siltstone configuration is ideal in that in a hydrostatic deformation mode, all particles experience the same deformation regardless of their original crystallographic orientation. Controlled, precise shock preservation experiments will provide valuable data on the particle-in-matrix model for quartz.

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