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Equation of state and evidence of enhanced phase transformation for shock compression of distended compounds

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ABSTRACT

Shear stress and deformation is inherent to shock-wave compression. Shear deformation is enhanced when the material subject to shock compression is in an initial distended state. Shock Hugoniot data for full-density and porous compounds of boron carbide, silicon dioxide, tantalum pentoxide, uranium dioxide and playa alluvium are investigated for purposes of equation-of-state representation of intense shock compression. Hugoniot data of distended materials reveal evidence of accelerated solid–solid phase transition as a consequence of shock compaction and accompanying enhanced shear deformation. A phenomenological thermo-elastic equation-of-state model is constructed that accounts for both deformation-induced phase transformation and the extreme shock compaction of distended solids, and applied to the compounds studied.

1. Introduction

Many compounds undergo solid–solid crystallographic phase transformation in the shock-wave environment. Forces leading to phase instability through the time history of the shock compression process are not well understood. Adequate shock pressure is certainly central to achieving phase transformation at the Hugoniot state. There is experimental evidence that shear stress and deformation also play a prominent role in the shock-induced phase transformation.

The underlying physics of shear in the acceleration of phase transformation in the shock environment is less clear. A state of shear can lead to localized shear deformation with attendant localized heating, mass diffusion, defect production and amorphization. Alternatively, or additionally, shear stresses will lead to distortional elastic strain energy that can lower energy barriers to crystal structure transformation.

Conditions that generate shear in the shock compression process are also complex. A homogeneous solid experiences shear in the uniaxial environment of the shock wave with the extent of shear stress, shear deformation, and elastic shear strain energy determined by the intensity of the shock and the crystal strength of the material. Granularity and crystal anisotropy will additionally amplify shock-induced shear. Shear in the shock compression event is further intensified when the initial material is distended (initially porous or powder state).

The interrelationship of shear deformation and molecular change of state in the shock-wave event has been pursued in earlier studies. Teller [1] speculated on the importance of shear in the chemical transformation within the shock wave. Although emphasis was on energetic reactions in the shock wave event, the physical arguments of Teller generally apply to the genesis of any molecular transformation in the shock process. Effects of shear deformation on the phase transformation under shock in silicate and carbonate minerals has been pursued with emphasis on underlying microscopic mechanisms [2].

In the present study shock Hugoniot data for high-strength compounds, including boron carbide, silicon dioxide, uranium dioxide and tantalum pentoxide, are all shown to exhibit features consistent with the influence of shear on the shock-induced phase transformation. The consequences of shear on the shock equation-of-state description of a solid are explored. A phenomenological equation-of-state model is developed that incorporates the enhancement of phase transformation brought about by shock compaction induce shear deformation and applied to the materials

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studied. The Rice–Walsh equation-of-state framework, rather than the more common Mie–Gruneisen equation of state, is employed and shown appropriate for the applications of concern. In particular, characterization is undertaken of the intense-pressure shock equation of state of moderate and highly distended solid compounds.

2. Shear and the shock phase transformation

Shear deformation is intrinsic to the shock compression event. There is both theoretical and experimental evidence that shear stresses and accompanying shear deformation augment the shock-induced phase transformation. Shock Hugoniot data for the compounds in this study provide evidence of the enhancement of phase transformation brought about by shock compaction and accompanying shear deformation. Recent diamond anvil cell (DAC) experiments and molecular dynamics calculations on boron carbide further supports the need for a shear component in initiating high-pressure phase transition in certain compounds.

Shock Hugoniot data for full density and 42% porosity α-quartz [3] are compared on the left in Fig. 1. Full density quartzite exhibits a Hugoniot elastic limit (HEL) strength of about 8 GPa [4]. Subsequent Hugoniot states traverse the mixed low and high pressure phase region, achieving complete transformation to the six-fold coordination stishovite phase at about 40 GPa. Hugoniot states for the porous α-quartz between 10 and 30 GPa reside substantially to the left (higher density) of the comparable-pressure full-density Hugoniot. Although at significantly higher temperature due to the excessive shock heating, increased densification of the porous quartz at comparable Hugoniot pressures suggests enhanced phase transformation brought about by the shock deformation process. Compressibility of the initial α-quartz phase is shown in the plot through a third-order Birch equation of state representation that is constrained by known elastic properties of the material. At the highest pressure the porous quartz Hugoniot resides to the right (lower density) of the fully density Hugoniot data due the different levels of shock heating and thermal expansion. The α-quartz-to-stishovite shock-induced phase transformation is reasonably well understood through numerous shock wave and DAC studies.

Similar behavior is exhibited by uranium dioxide in the center plot where Hugoniot states for nominally 6% porous and 42% porous UO_2 are compared [5]. Phase transformation on the solid material Hugoniot is less conclusive than that for SiO_2. Gust [6] proposes a Hugoniot transformation in the range of 44–54 GPa. DAC studies report transformation in UO_2 between about 33 and 40 GPa [7]. Again, Hugoniot states between about 10 and 40 GPa for the porous UO_2 reside at markedly higher density states, indicative of enhanced phase transformation under shock compression. Again, initial phase compressibility is described by a third-order Birch equation of state.

A similar plot is shown on the right comparing near-full density (3–7% porosity) boron carbide with more porous (22–25%) B_4C. Pressure-induced phase transformation in boron carbide is uncertain, although detailed analysis of shock Hugoniot data [8] and DAC studies [9] are suggestive of a solid–solid phase transition. Enhanced compression, and possibly phase transformation, of the more porous boron carbide within the lower-pressure Hugoniot regime is indicated by the Hugoniot data, although less definitive than the behavior of SiO_2 and UO_2.

The shock Hugoniot data contrasting near-full-density and distended samples of the same compounds shown in Fig. 1 collectively support the effects of enhanced Hugoniot compressibility with increasing distention. Possible incomplete compaction at the Hugoniot state would further amplify the difference. The proximity with known or suspected phase transformation on the Hugoniot supports increasing phase transformation with increasing shock deformation associated with the initial state of distention. A Birch third-order equation of state based on known compressibility properties of the initial crystal state is shown in the plots for the three compounds. The increased densification on the Hugoniot of all the data within the range of comparison further supports shock induced phase transformation.

Further support for shear deformation enhanced phase transformation is provided by the study of Yan et al. [9] on boron carbide. DAC hydrostatic compression of single crystal B_4C reveals uniform compression of B_4C to 60 GPa with no evidence of amorphous phase associated with high-pressure phase transformation. The same DAC test conducted with a hard granular pressure-transmitting medium (PTM) leads to extensive amorphization of boron carbide. Amorphization is reported to be a consequence of nonhydrostatic stress and deformation brought about by the granular PTM. Supporting molecular dynamics (MD) calculations of compression of the boron carbide unit cell consisting of a rhombohedra array of $B_{11}C$ icosahedra with a cross-linking C–B–C chain suggests sensible molecular mechanisms leading to the observed pressure- and deformation-induced amorphization. Hydrostatic compression in excess of 60 GPa yields self-similar compression of the unit cell. Nonhydrostatic uniaxial compression of the unit cell leads to deformation instability and lattice structure transformation (phase transformation) in the 19–23 GPa pressure range with a 4% density increase.

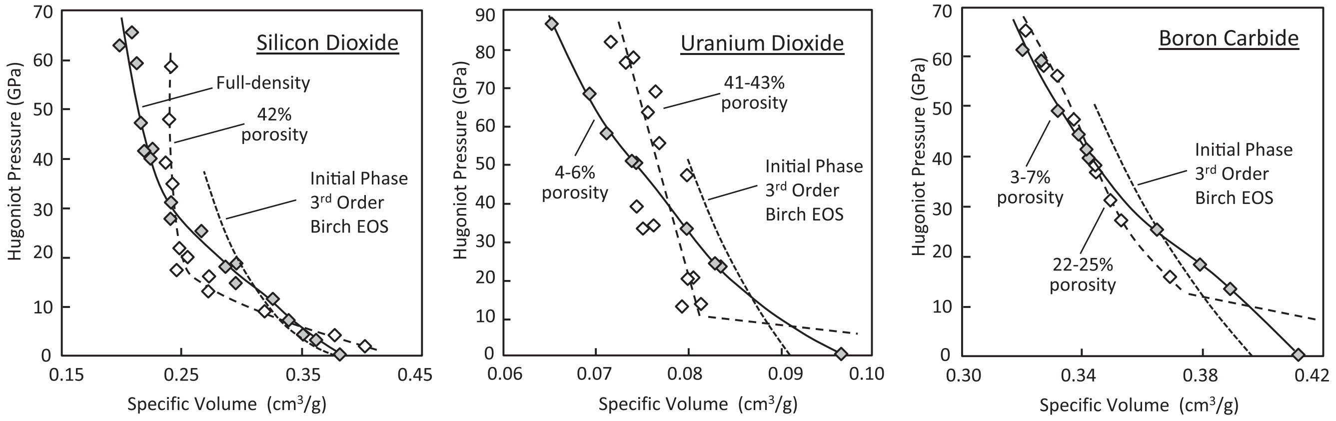

Fig. 1. Comparison of Hugoniot states for near-full-density material (solid points) and porous material (open points) illustrating increased compressibility at lower shock pressures for the more distended material. Data suggests phase transformation is enhanced by increased deformation of the more porous material. Third-order Birch equation of state representation of initial phase compressibility reveals increased Hugoniot densification for the three materials.