

NMR SPECTROSCOPIC ANALYSIS OF EXPERIMENTALLY SHOCKED QUARTZ AND THE FORMATION OF DIAPLECTIC GLASS\* M. B. Boslough<sup>1</sup>, R. T. Cygan<sup>1</sup>, R. J. Kirkpatrick<sup>2</sup>, and B. Montez<sup>2</sup>, <sup>1</sup>Sandia National Laboratories, Albuquerque, New Mexico 87185 and <sup>2</sup>University of Illinois, Urbana, Illinois 61801

The shock-loading of natural materials by impact can result in the formation of highly modified and altered phases. Shocked minerals typically exhibit fracturing, planar deformation, disordering, glass formation, and/or polymorphic phase transformations which depend upon the peak pressures and temperatures (1,2). Diaplectic glasses, which are presumed to form during the shock event, often occur at moderate to large shock pressures (above 5 GPa). Coesite and stishovite, crystalline polymorphs of silica, have been observed to form at higher shock pressures, although trace and minor amounts of both have been detected in samples from pressures below 15 GPa (2).

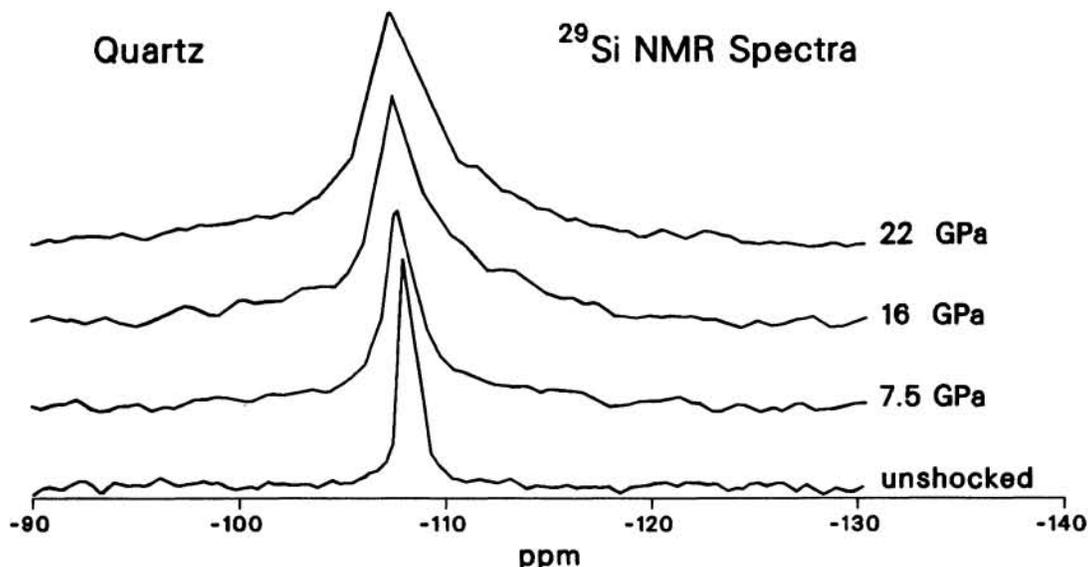
Shock-modified minerals and glasses from natural impacts and from shock experiments have been subjected to a variety of physical property analyses in earlier studies. For example, optical and electron microscopy have been used to examine various structural shock features, while refractive index and density measurements have been used to determine properties of individual phases. X-ray diffraction has detected the presence of minor phases, and, along with electron spin resonance measurements, has provided information on shock-induced lattice disorder. Recently, <sup>29</sup>Si nuclear magnetic resonance (NMR) spectroscopy has been successfully used to identify and determine the ratio of coesite to stishovite in shocked sandstone obtained from a terrestrial impact crater (3). This sensitive technique can detect the presence of trace amounts of the SiO<sub>2</sub> polymorphs as well as silica glass that may have formed during shock compression. Solid state NMR spectroscopy is well-suited for analyzing natural or synthetic shock products and, with the pulse Fourier transform method, complements the other analytical methods in detecting and characterizing the effects of shock-loading upon quartz. The NMR experiment measures radio-frequency emissions from nuclei which have been excited to higher energy states by electromagnetic pulses while the sample is located in a very strong magnetic field. The magic-angle sample spinning (MASS) method significantly reduces part of the peak broadening effect associated with solid state NMR, thereby improving the spectral resolution.

In the present study we have used <sup>29</sup>Si NMR spectroscopy to examine the products recovered from the experimental shock-loading of pure synthetic quartz powders to mean peak pressures of 7.5 to 22 GPa. Our purpose was to measure the changes in quartz disorder and diaplectic glass formation as a function of shock pressure, in addition to determining the existence of minor high-pressure crystalline phases. The shock experiments were performed using the Sandia "Bear" explosive loading fixtures to achieve well-characterized shock states. Mean bulk shock temperatures were estimated from numerical calculations based upon the fixture geometry and the initial sample density (4). These temperatures range from 350°C at 7.5 GPa to 600°C at 22 GPa. Approximately 200-300 mg of shocked powder recovered from each sample fixture were used to obtain the <sup>29</sup>Si NMR spectra.

The accompanying figure provides the MASS NMR spectra of the unshocked starting material (pure quartz at 1.3 g/cm<sup>3</sup>) and the recovered samples shocked to various mean peak pressures. The NMR resonance frequency is provided in units of ppm relative to an external standard. At a given frequency, the intensity of emission is proportional to the population of <sup>29</sup>Si nuclei whose local environment yields that resonance. The chemical shift (in ppm)

quantifies the extent of electronic shielding for that environment. The unshocked quartz is characterized by a single narrow resonance at about -108 ppm, but with increasing pressure, this peak broadens and spectral intensity develops in the -110 to -120 ppm range. This intensity increases with increasing shock pressure. We believe the broadening of the quartz peak is due to disorder (defects, dislocation, damage, and residual strain) in the quartz lattice. The broad secondary peak (-110 to -120 ppm) is consistent with that of 4-fold coordinated silicon in SiO<sub>2</sub> glass (5). Spectra obtained using shorter, 5 sec, recycle times contain relatively more signal for the glass, consistent with previous results (3). There is no evidence of 6-fold coordinated silicon, which resonates in the -190 to -200 ppm range. We have performed best-fit Gaussian simulations of each NMR spectrum in order to resolve and quantify the contributions of each resonance to the spectrum, thereby providing relative abundances of the glass and quartz phases from comparison of integrated peak areas.

We believe the systematic broadening of the quartz resonance with shock pressure may provide a sensitive calibration for determination of peak pressures in naturally shocked quartz. Potential applications of this method include the determination of peak shock pressure decay as a function of distance from an impact or nuclear explosion site, and the quantitative measurement of shock effects in quartz grains concentrated from the clay layer of the Cretaceous-Tertiary boundary.



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