Supplementary data

Acoustic shock waves induced sp^2-to-sp^3 type phase transition: A case study of graphite single crystal

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Shock wave loading experiment

The required shock waves have been generated by an in-house tabletop semiautomatic shock tube which has three sections known as driver, driven and diaphragm sections that are made of seamless steel. The driver and driven sections consist of long tubes of 48 cm and 180 cm, respectively and both have an inner diameter of 1.5 cm. Atmospheric air is used as the input source for the required shock wave generation. While the atmospheric air is compressed into the driver section, at the critical pressure, the diaphragm ruptures and the shock wave is generated and moves along the driven section. The detailed mechanism and working methodology of the pressure-driven shock tube are discussed in the previous publication. For the present experiment, the shock waves of Mach number 2.2 with the reflected transient pressure of 2.0 MPa (P_5) and the transient temperature of 864 K (T_5) have been used and the values have been calculated by the standard R-H relations as in equations (1-4).

$$P2 = P1\left[1 + \frac{2\gamma}{\gamma + 1}(M^2 - 1)\right] \text{..... (1)}$$

$$\frac{T_2}{T_1} = \frac{P_2}{P_1}\left[\frac{\left(\frac{\gamma + 1}{\gamma - 1}\right) + \frac{P_2}{P_1}}{1 + \left(\frac{\gamma + 1}{\gamma - 1}\right)\frac{P_2}{P_1}}\right] \text{..... (2)}$$

$$\frac{P_5}{P_2} = \frac{(3\gamma - 1)\frac{P_2}{P_1} - (\gamma - 1)}{(\gamma - 1)\frac{P_2}{P_1} + (\gamma + 1)} \text{..... (3)}$$

$$\frac{T_5}{T_2} = \frac{P_5}{P_2}\left[\frac{\left(\frac{\gamma+1}{\gamma-1}\right)+\frac{P_5}{P_2}}{1+\left(\frac{\gamma+1}{\gamma-1}\right)\frac{P_5}{P_2}}\right] \quad \ldots\ldots\ldots (4)$$

The initial fixed values are P_1 = 1 bar, $\gamma = 1.4$, T= 300 K, where M- Mach number, P5 and T5 are the reflected transient pressure and temperature at the end of the driven tube.

The test samples have been placed one by one with the required interval between them in the sample holder which is typically placed 1cm away from the open end of the shock tube. Subsequently, 1, 2, 3, 4, 5 and 500 shock pulses have been loaded on the respective test samples with an interval of 5 s between each shock pulse. For example, 5 pulses mean shock wave exposed on a sample 5 times with Mach number 2.2 (±0.1). After the completion of the shock wave loading, the control and shock wave-loaded samples have been analyzed by Raman, XPS, and TEM studies so as to understand the effect of shock waves on graphite crystals.

Analytical instrument details

Raman Spectroscopy Experiment

We investigated the Raman spectra of the control and shocked graphite samples using a Renishaw 2000 micro confocal Raman spectrometer coupled with a 532 nm argon ionic excitation source. Single-crystal silicon with a characteristic Raman peak at 520.0 cm^{-1} was utilized to calibrate the Raman spectroscopy system prior to measurement. Raman spectra of the control and shocked graphite samples were gathered within the wavenumber range of 100−3500 cm^{-1} in the backscattering geometry with the spectral resolution of 1.0 cm^{-1} and the acquisition

time was 120 s. The laser spot size was 50 μm^2 and the optical microscope's objective lens was used such that an X50 long working distance objective lens (WD = 10.6 mm) was utilized and the value of numerical aperture was 0.5 while the Raman data was collected by Renishaw Wire 5.1 instrument control and the data acquisition software. We processed the obtained Raman spectra with a Lorentzian-type function in Origin 9.0 software to extract the Raman peak position and its corresponding FWHM.

X-ray Photoelectron Spectrometer Experiment

We investigated the carbon bonding patterns of the control and shocked graphite crystals by XPS analysis. For this study, PHI - VERSAPROBE III – X-ray Photoelectron spectrometer was utilized. The typical characteristics of the spectrometer are as follows: Monochromatic X-ray Beam area is 15 μm and Al Kα radiation (1486.6 eV) and the data was recorded over the input energy from 0-1350 eV. The single crystals of the control and shocked graphite were utilized as it is to record the XPS data. XPS spectra were deconvoluted with CasaXPS 2.3.12 software, using a non-linear least squares fitting routine after a Shirley-type background subtraction and the peaks were interpreted using a combination of Gaussian/Lorentzian functions. The adjusted parameters were FWHM, binding energy and peak area. To correct possible deviations caused by the electric charge of the samples, the C1s band at 284.6 eV was taken as the internal standard. Surface atomic percentages were calculated from the corresponding peak areas upon spectra deconvolution and using the sensitivity factors provided by the manufacturer.

HR-TEM Experiment

Microscopical structural characterizations for the starting and 500 shock-recovered samples were investigated using HRTEM, which was operated at the State Key Laboratory of Environmental Geochemistry, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, China. A small amount of sample was homogeneously distributed onto a carbon-film-coated copper grid for the HRTEM observation, which was performed through a Tecnai G2 F20 S-TWIN TMP with an acceleration voltage of 200 kV. We precisely measured the interplanar spacing of the samples through the Image J software.