Chapter 5

Hypervelocity Impacts of Macroscopic Bodies

5.1 Asteroid impacts on the Earth

Although the Earth is constantly bombarded with small meteorites and micrometeorites, large impacts are (thankfully) infrequent. Still, such impacts have taken place on several occasions [1]. One major impact occurred 65 million years ago at the Cretaceous-Tertiary (K-T) Boundary [2]. The fossil record of this time shows an extinction of more than half the marine and land biota, including dinosaurs, marine and flying reptiles, and numerous microscopic genera. It is believed that this mass extinction was caused by the impact of an asteroid on the Yucatan Peninsula, Mexico, known as the Chicxulub impact event [3].

The Chicxulub asteroid was approximately 10 km in diameter and impacted at a velocity of roughly 20 km/s [4]. The resulting crater is buried, but has been estimated to span nearly 300 km [5]. The geology of this region consists of a 3 km thick calcium carbonate layer containing significant calcium sulfate in the form of gypsum and anhydrite [6].
Several reasons have been put forward to explain the mass extinction associated with the Chicxulub impact. First, the ejected dust may have reduced the levels of sunlight reaching the Earth to such an extent that photosynthesis halted for a period of time [2]. Second, carbon dioxide released from carbonates upon impact may have caused global warming [1]. Third, acid rain may have resulted from the production of nitric acid as the atmosphere was heated during impact [7]. Finally, the release into the atmosphere of sulfur oxides, SO₂ and/or SO₃, from gypsum and anhydrite during impact may have caused global cooling or acid rain [3]. All of these events may have caused significant global changes and the extinction of many species.

The sulfur oxide scenario has been the subject of much interest. The amount of sulfur-bearing gas evolved during the Chicxulub impact has been estimated to be between $5 \times 10^{16}$ g and $5 \times 10^{18}$ g [4]. Two reaction mechanisms have been proposed [8, 9] for the shock-induced conversion from calcium sulfate to sulfur oxides in a Chicxulub-type impact:

$$2\text{CaSO}_4 \rightarrow 2\text{CaO} + 2\text{SO}_2 + \text{O}_2$$  \hspace{1cm} (1)

$$\text{CaSO}_4 \rightarrow \text{CaO} + \text{SO}_3.$$  \hspace{1cm} (2)

Note that the sulfur oxide product is different in each mechanism. Theoretical treatments and experimental results are inconclusive as to which mechanism predominates under Chicxulub-type impact conditions [9]. Models to predict the consequences of sulfur oxides on the K-T extinction are complicated not only by large uncertainties in the vaporization mechanism (and hence, the species of sulfur oxide produced), but also by large uncertainties in the quantities of vapor released in the impact. As such it is not possible to say with reasonable certainty whether or not the
evolution of sulfur oxides was a major contributing factor in the K-T extinction. The importance of evolved carbon dioxide is similarly uncertain [6].

5.2 Description of mass spectrometer to study shock-induced vaporization and ionization of minerals

In order to characterize the chemical mechanisms involved in impact-vaporization of sulfur-bearing minerals, I designed a time-of-flight mass spectrometer capable of detecting vapor produced at the surface of a shocked mineral sample. This instrument will be used to study the relationship between impact parameters and the resulting sulfur oxides, providing critical experimental evidence for the role of sulfur oxides in the global climate change and mass extinction at the K-T Boundary.

In designing a mass spectrometer for analysis of shock-induced vapor, several points were given consideration. First of all, impacts would be generated using a fast projectile, which would likely disrupt the mass spectrometer vacuum system. A projectile would break vacuum, crush electrostatic grids, and short the electrical systems responsible for ion extraction and focusing. The mass spectrometer must be designed in such a way that the vaporized materials would be ionized, extracted, and analyzed faster than the projectile or atmospheric gases could interfere.

Another consideration was the ionization method. Some molecules would be ionized during the impact process itself. These could be extracted and analyzed as is. Other molecules would be evolved as neutrals, and would need to be ionized prior to extraction and analysis. In distinguishing between evolved SO$_3$ and SO$_2$, it would
necessary to take every precaution to avoid fragmentation during ionization. In addition, quantitative analysis required a method for which ionization cross-sections would be similar for all species of interest. Electron impact ionization was chosen over multiphoton ionization for this purpose.

Given the uncertainties in the duration of impact vaporization, two methods of ion extraction are possible. The ionizing electron beam could be pulsed; however, there is some uncertainty in the timing of the pulse relative to vapor formation. The other option is to use a continuous electron beam and subsequently pulse the ion extraction field. Although both options are viable, it was decided to use pulsed orthogonal extraction to sample ions. Ions then travel through a drift tube and an optional reflectron and are analyzed using a continuous dynode detector.

Figure 5.1 shows the experimental setup for these studies. Figure 5.2 shows an enlargement of the mass spectrometer section of the experimental setup. Figure 5.3 shows details of the electrodes and grids used to produce and extract ions. A projectile is launched toward the mass spectrometer. The projectile strikes a driver plate, onto which the mineral sample is mounted. As the shock wave travels through the mineral and reaches the free surface, vapor and ions are produced. One or more skimmers and apertures reduce the quantity of ejecta produced, according to the limitations of the ion optics and the ion detector. The attenuation of the electron beam, as measured by the faraday cup, will indicate the quantity of neutrals remaining. For studies of neutral species, ions formed by the shock wave are repelled by biasing the skimmers and/or apertures with +400 V. For studies of ions produced by the shock wave, the electron
Figure 5.1. Experimental setup for shock-induced vaporization mass spectrometry experiments. Projectiles are fired from a hypervelocity gun. Other projectile sources can also be used. The projectile impacts a driver plate, which transmits a shock wave to a mineral sample mounted inside the time-of-flight orthogonal extraction reflectron mass spectrometer. Vapor molecules are ionized using an electron gun, then extracted and analyzed. Although vacuum is compromised, ions are extracted fast enough to prevent interference. The next page shows an enlargement of the mass spectrometer region.
Figure 5.2. Details of the mass spectrometer system. Impact of the projectile on the mineral produces both ions and neutrals. Skimmers reduce the neutral density to an appropriate amount for electron impact ionization. Ions are collimated when they enter the pulsed extraction region. Lenses between the electron beam and the pulsed extraction region allow control over energy profile. Ions are pulsed into the reflectron chamber, where they are analyzed by an electron multiplier.
Figure 5.3. Electrodes and lenses involved in ion formation and extraction.
beam is simply turned off and the skimmer voltages are biased according to the ions being studied (negative to extract positive ions, positive to extract negative ions).

Neutral species are ionized by the electron beam, which is placed as close as practical to the mineral sample. The resulting ions are extracted by the voltage in the ionization region, and further extracted by the grid of the collimating lenses. Total ion energy at this point should be around 100-300 V. Although orthogonal extraction is typically performed using smaller voltages [10], ions in this experiment must be extracted and analyzed quickly to avoid contamination and destruction of the mass spectrometer by the projectile. For the experiment originally envisioned (20 mm projectile at several km/s), the projectile continues its forward motion after impact with the driver plate. If vacuum breaks, the inrush of atmospheric gases poses significant problems, but not for a few microseconds. In addition, as the projectile continues to move forward, electrostatic lenses, skimmers, and other components will be destroyed. The ion extraction technique presented here will be faster than these interferences. Of course, non-projectile methods of producing shock waves in minerals can be used with smaller extraction voltages, and with much fewer complications.

Mass resolution in an orthogonal extraction instrument is dependent on the degree of collimation of the ion trajectories as they travel through the orthogonal extraction region (before the push-out pulse) [11]. Collimating lenses are used for this purpose. When ions reach the extraction region, a pulse is applied to push the ions into the drift tube. Dual stage extraction at this point serves to compensate for the spread in the ion beam in the orthogonal extraction region. Ions travel through the drift tube to the
detector. A reflectron may be needed to achieve high mass resolution, but might not be needed for lower resolution experiments.

Orthogonal extraction is used only with continuous ion sources, or at least with ion sources that vary in time in a predictable way. In this case, the vapor produced at the mineral surface certainly has a strong time-dependence. Ions are formed as they reach the electron beam. However, the time history of vapor formation, the distribution of initial kinetic energies of vapor molecules, and the velocities of ions with different m/z will all affect the time-dependent homogeneity of the ions in the orthogonal extraction region. This must be taken into account when analyzing the data. It may be possible to probe the time dependence of mineral vaporization using repeated experiments.

Quantitative analysis of speciation must take this factor into account. For instance, say species X is produced immediately upon impact, while an equal quantity of species Y is produced a short time later. If the orthogonal extraction pulse takes place early, more of species X is observed. If the pulse is later, species Y appears to be dominant. Studying the results from several pulse delays will give the time history of X versus Y, but a single spectrum will be misleading with respect to the total amount of each that was originally formed. Similarly, species X and species Y may be formed at the same time and with the same kinetic energy, but if species X is lighter than species Y, it will arrive in the orthogonal extraction region first. This mass effect can be taken into account only if many spectra are taken using several different pulse delay times.

Although shocked mineral experiments have not yet begun, assembly of the mass spectrometer is nearing completion. Initial experiments will use small detonation-type devices to produce the shock wave in various mineral samples. Although the
corresponding impact velocities are slow, detonation-type shocks allow repeated measurements on the same sample. Projectiles from a light gas may be used in further experiments when the required impact velocities are larger.

5.3 References


