Fall 2013

The Formation of Distal Impact Ejecta

Brandon C. Johnson

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Entitled
THE FORMATION OF DISTAL IMPACT EJECTA

For the degree of Doctor of Philosophy

Is approved by the final examining committee:
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Head of the Graduate Program Date
THE FORMATION OF DISTAL IMPACT EJECTA

A Dissertation
Submitted to the Faculty
of
Purdue University
by
Brandon C. Johnson

In Partial Fulfillment of the
Requirements for the Degree
of
Doctor of Philosophy

December 2013
Purdue University
West Lafayette, Indiana
I dedicate this dissertation to my amazing wife Alexandria who kept me sane during the past half decade, to my undergraduate advisor Ranjit Pati who convinced me to pursue an advanced degree, and to my parents without whom I surely would not be where I am today.
ACKNOWLEDGEMENTS

I am very grateful for my advisor H. Jay Melosh who taught me how to be a scientist. I thank Jay for the opportunity to see the Sudbury impact structure and its ejecta layer nearly 800 km away. The field trip to the Sudbury ejecta, my first field experience, helped me realize the importance of geologic observations. I must also thank Jay for the field trip he lead to Kentland crater in Indiana, allowing me to attend many scientific conferences, and giving me the chance to see the unforgettable launch of the GRAIL mission’s twin spacecraft.

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I also thank Casey Lisse. Together we worked to understand a system called HD 172555, which has a dusty debris disk created by a planetary scale hypervelocity impact (Johnson et al. 2012). Without Casey, I would have never seen the (infrared) light.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>LIST OF TABLES</th>
<th>vii</th>
</tr>
</thead>
<tbody>
<tr>
<td>LIST OF FIGURES</td>
<td>viii</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>xi</td>
</tr>
<tr>
<td>CHAPTER 1. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>CHAPTER 2. DISTAL IMPACT EJECTA</td>
<td>6</td>
</tr>
<tr>
<td>2.1 Tektites</td>
<td>6</td>
</tr>
<tr>
<td>2.2 K-Pg Boundary Layer</td>
<td>10</td>
</tr>
<tr>
<td>2.3 Other Ejecta Layers</td>
<td>15</td>
</tr>
<tr>
<td>2.3.1 Evidence to support an impact origin</td>
<td>15</td>
</tr>
<tr>
<td>2.3.1.1 Impact Spherules</td>
<td>16</td>
</tr>
<tr>
<td>2.3.1.2 Isotopic Data</td>
<td>17</td>
</tr>
<tr>
<td>2.3.1.3 Shocked Quartz</td>
<td>19</td>
</tr>
<tr>
<td>2.3.2 Ejecta Layers as Record of Impacts</td>
<td>20</td>
</tr>
<tr>
<td>CHAPTER 3. FORMATION OF SPHERULES IN IMPACT PRODUCED VAPOR PLUMES</td>
<td>28</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>29</td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
</tr>
<tr>
<td>---------</td>
<td>-------</td>
</tr>
<tr>
<td>3.2</td>
<td>Methods</td>
</tr>
<tr>
<td>3.3</td>
<td>Results</td>
</tr>
<tr>
<td>3.3.1</td>
<td>Spherule Formation</td>
</tr>
<tr>
<td>3.3.2</td>
<td>Expansion</td>
</tr>
<tr>
<td>3.3.3</td>
<td>Nucleation</td>
</tr>
<tr>
<td>3.3.4</td>
<td>Growth and Quenching</td>
</tr>
<tr>
<td>3.3.5</td>
<td>Spatial/Temporal Dependence</td>
</tr>
<tr>
<td>3.3.6</td>
<td>Impactor Size and Velocity Dependence</td>
</tr>
<tr>
<td>3.4</td>
<td>Discussion</td>
</tr>
</tbody>
</table>

Appendix: Details of Nucleation and Chemistry | 69 |
| A.1 | Homogeneous Nucleation and Growth | 69 |
| A.2 | Numerical Solution of Nucleation Equations | 73 |
| A.3 | Surface Energy | 77 |
| A.4 | Vapor Phase Chemistry | 79 |
| A.5 | Kinetically Frustrated Nucleation | 81 |

CHAPTER 4. IMPACT SPHERULES AS A RECORD OF AN ANCIENT HEAVY BOMBARDMENT OF EARTH | 83 |

CHAPTER 5. FORMATION OF MELT DROPLETS, MELT FRAGMENTS, AND ACCRETIONARY IMPACT LAPILLI DURING A HYPERVELOCITY IMPACT. | 95 |
<p>| 5.1 | Introduction | 96 |
| 5.2 | Results | 105 |
| 5.2.1 | Detailed Model of the Ejecta Curtain | 107 |</p>
<table>
<thead>
<tr>
<th>Table</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 2.1 Craters Larger than 85 km in Diameter</td>
<td>27</td>
</tr>
<tr>
<td>Table 3.1 Initial Conditions of Vapor Plumes</td>
<td>41</td>
</tr>
<tr>
<td>Table 4.1 The Earth’s Impact History From Spherule Layer Data</td>
<td>88</td>
</tr>
<tr>
<td>Table 5.1 iSALE Input Parameters (Barringer Release)</td>
<td>101</td>
</tr>
<tr>
<td>Table 5.2 Observations of Average Spherule Size</td>
<td>127</td>
</tr>
<tr>
<td>Table 5.3 Observations of Average Sizes of Accretionary Impact Lapilli</td>
<td>135</td>
</tr>
</tbody>
</table>

Appendix Table

<table>
<thead>
<tr>
<th>Table</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table B.1 Compiled Tracer Data</td>
<td>146</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure 2.1 Probability of Crater Survival on Earth</td>
<td>21</td>
</tr>
<tr>
<td>Figure 2.2 Total Number of Craters Larger than 85 km in Diameter on Earth</td>
<td>23</td>
</tr>
<tr>
<td>Figure 2.3 Number of Surviving Craters Larger Than 85 km in Diameter on Earth</td>
<td>26</td>
</tr>
<tr>
<td>Figure 3.1 Release Adiabats</td>
<td>32</td>
</tr>
<tr>
<td>Figure 3.2 Vapor Plume Cartoon</td>
<td>40</td>
</tr>
<tr>
<td>Figure 3.3 Normalized Cell Velocity</td>
<td>43</td>
</tr>
<tr>
<td>Figure 3.4 Adiabatic Paths Showing Nucleation, Growth, and Quenching</td>
<td>45</td>
</tr>
<tr>
<td>Figure 3.5 Detail of Nucleation Event in Density-Temperature Space</td>
<td>47</td>
</tr>
<tr>
<td>Figure 3.6 Degree of Supercooling During Nucleation</td>
<td>49</td>
</tr>
<tr>
<td>Figure 3.7 Spherule Size Distribution in Cell 80</td>
<td>51</td>
</tr>
<tr>
<td>Figure 3.8 Time of Nucleation versus Location in the Plume</td>
<td>53</td>
</tr>
<tr>
<td>Figure 3.9 Spherule Diameter versus Location in the Plume</td>
<td>54</td>
</tr>
<tr>
<td>Figure 3.10 Spherule Size Distribution in Plume</td>
<td>58</td>
</tr>
<tr>
<td>Figure 3.11 Average Spherule Diameter versus the Inverse of the Rate of Change of the Degree of Supercooling</td>
<td>59</td>
</tr>
<tr>
<td>Figure 3.12 Number of Spherules Depends as a Function of the Rate of Change of the Degree of Supercooling</td>
<td>59</td>
</tr>
<tr>
<td>Figure</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>------</td>
</tr>
<tr>
<td>Figure 3.13 Average Spherule Size Created by Different Impact Conditions</td>
<td>62</td>
</tr>
<tr>
<td>Figure 3.14 Condensed Mass as a Function of Impact Velocity</td>
<td>63</td>
</tr>
<tr>
<td>Figure 4.1 Estimate of Impact Velocity for Layer S1</td>
<td>89</td>
</tr>
<tr>
<td>Figure 4.2 The Earth's Impactor Size Frequency Distribution</td>
<td>94</td>
</tr>
<tr>
<td>Figure 5.1 Release Adiabats and Liquid Vapor Coexistence Curve</td>
<td>99</td>
</tr>
<tr>
<td>Figure 5.2 Impact Time Series</td>
<td>100</td>
</tr>
<tr>
<td>Figure 5.3 Ejecta Curtain Cartoon</td>
<td>106</td>
</tr>
<tr>
<td>Figure 5.4 Density Change During Release</td>
<td>110</td>
</tr>
<tr>
<td>Figure 5.5 Peak Shock Pressure</td>
<td>112</td>
</tr>
<tr>
<td>Figure 5.6 Ejection Velocity</td>
<td>113</td>
</tr>
<tr>
<td>Figure 5.7 Peak Shock Pressure versus Ejection Velocity</td>
<td>115</td>
</tr>
<tr>
<td>Figure 5.8 Mass Ejected versus Ejection Velocity</td>
<td>117</td>
</tr>
<tr>
<td>Figure 5.9 Provenance Map of Ejection Velocity</td>
<td>119</td>
</tr>
<tr>
<td>Figure 5.10 Melt Fragment Size as a Function of Ejection Velocity</td>
<td>122</td>
</tr>
<tr>
<td>Figure 5.11 Melt Droplet Diameter as a Function of Ejection Velocity</td>
<td>126</td>
</tr>
<tr>
<td>Figure 5.12 Accretionary Impact Lapilli Diameter as a Function of Ejection Velocity</td>
<td>134</td>
</tr>
</tbody>
</table>

**Appendix Figure**

<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure A.1 Illustration of 1-D Lagrangian Hydrocode</td>
<td>74</td>
</tr>
<tr>
<td>Figure A.2 Surface Energy versus Temperature</td>
<td>78</td>
</tr>
<tr>
<td>Figure A.3 Spherule Diameter versus Impact Velocity for Transition Temperatures</td>
<td>79</td>
</tr>
<tr>
<td>Figure B.1 Pressure as a Function of Time for One Tracer</td>
<td>143</td>
</tr>
</tbody>
</table>
Appendix Figure

| Figure B.2 Velocity as a Function of Time for One Tracer. | 144 |
| Figure B.3 Acceleration as a Function of Time for One Tracer. | 145 |
| Figure B.4 Geometry of Ejecta Curtain. | 148 |
ABSTRACT


Here we present two models for the dynamics of ejection and formation of distal impact ejecta. The first model focuses on the most highly shocked material that forms a massive expanding vapor plume or fireball. In this model molten droplets or spherules condense from the vapor. We model the expanding vapor plume using a one dimensional Lagrangian hydrocode. The condensation of droplets is treated by directly coupling the equations for homogeneous nucleation and growth with our hydrocode. The second model is focused on less energetic material ejected as part of the excavation flow. Using the iSALE hydrocode, we determine the details of the excavation flow and formation of the ejecta curtain. Using this information and some simple analytical approximations we produce a model for the formation of melt droplet spherules, melt fragments, and accretionary impact lapilli, within this flow.

Using our model for spherules produced in the vapor plume, we create a method to estimate the size of an impactor and impact velocity required to create a spherule layer. The impactor size depends on the thickness of the layer and the impact velocity depends on the size of the spherules within the layer. Using observations of known spherule layers...
and the derived dependence on impactor size, we show that the impactor flux on Earth was significantly higher \( \sim 2 - 3.5 \) Gyr ago than it is today. Our model for the less energetic material ejected as part of the ejecta curtain predicts how ejecta particle sizes depend on impactor size and ejection velocity. In the future, this model can also be used to estimate the scale of an impact required to make observed distal impact ejecta layers.
CHAPTER 1. INTRODUCTION

When an extraterrestrial body strikes the Earth, a shock wave propagates from the point of impact, accelerating the target material and decelerating the projectile. During the impact roughly half of the impact energy is converted to thermal energy, resulting in the melting and vaporization of rock. The vaporized material expands as a massive vapor plume or fireball and melted material is ejected as part of the excavation flow, forming an ejecta curtain as the crater continues its growth. For large impacts this ejected material can be found as layers in the geologic record far from the source crater. The study of these distal ejecta layers has focused on geochemistry and geologic observations while the physical details of the formation of distal impact ejecta layers have received little attention (Koeberl 1986).

Within these layers, sub-millimeter to millimeter scale previously molten droplets called spherules are found (Simonson and Glass 2004). In addition to these spherules, cm scale previously molten particles called tektites, melt clasts, or blebs (Koeberl 1986, Pufahl et al. 2007, Smit 1999) and accretionary particles similar to volcanic accretionary lapilli (Schulte et al. 2010) are also found. The present work is focused on understanding the dynamics of ejection and the formation of these various ejecta particles.
Undoubtedly, distal impact ejecta layers preserve a record of the impacts that formed them. On Earth, where craters are quickly destroyed or obscured by tectonics and weathering, impact ejecta layers may be the only evidence that remains to indicate a massive impact occurred. By understanding the processes that create these layers and the various particles within, we hope to gain valuable information about the impacts that created the layers. Models that describe the formation of distal ejecta layers may indicate how certain layer properties depend on impactor size, ejection velocity, or impact velocity. Such a dependence and appropriate geologic observations may allow us to determine the impact conditions even when a source crater cannot be found.

In Chapter 2 I describe the long history of interest in these distal impact ejecta layers. We begin the chapter with a discussion of tektites and the eventual realization that tektites are the product of terrestrial impacts. Then I focus on the K-Pg boundary layer as this is the most studied ejecta layer, which has been found at over 350 unique sites across the globe. The K-Pg boundary is especially interesting because, up to ~5000 km from the source crater, the boundary has a distinct two-layer structure. The upper layer is thought to be the product of a massive vapor plume or fireball while the underlying layer found nearer to the source crater comes from the less energetic ejecta curtain. Next I discuss other distal ejecta layers, including an expanded description of the lines of evidence used to argue for a layer’s impact origin. I end Chapter 2 with a description of the information I hope to gain from studying distal impact ejecta, namely the size of the impactors that created these layers and to motivate the importance of understanding the Earth’s impact chronology.
In Chapter 3 (reprinted from Icarus, Volume 217, B. C. Johnson and H. J. Melosh, Formation of spherules in impact produced vapor plumes, 416-430, Copyright (2012), with permission from Elsevier.) we construct a numerical model of spherule formation in an impact produced vapor plume. This model tracks the expansion of the vapor plume using a one-dimensional Lagrangian hydrocode coupled with the ANEOS equation of state for silica. We then include the equations for nucleation and growth as described by homogeneous nucleation theory to describe the process of spherule formation. We use this model to determine the number and size of the spherules that an impact creates. We also explore when and where spherules are formed in the vapor plume, and how this affects the size of the spherules. In general we find that smaller spherules form in the outer, faster moving, portions of the vapor plume at earlier times. This work also explores the effect of impactor size and impact velocity on the resultant spherule size. We report a simple linear dependence on impactor size and a complex dependence on impact velocity. We find that a 10 km diameter asteroid impacting at a velocity of ~21 km/s creates spherules that are ~250 μm in diameter, which is comparable to the spherules found in the K/Pg boundary layer.

Based on the results described in Chapter 3, we develop a simple model used to estimate the size of an impactor that created a given global fireball layer based solely on the thickness of the layer (Chapter 4, reprinted from Nature, 485, B. C. Johnson and H. J. Melosh, Impact spherules as a record of an ancient heavy bombardment of Earth, 75-77, Copyright (2012), with permission from Brandon Johnson.). This model also gives estimates of the impact velocity based on the average size of the spherules within the
layer. Using this model and geologic observation of known spherule layers we are able to produce the first impactor size-frequency distribution for Earth, that is not based on the incomplete impact chronology of the Moon or estimates of the current day impactor flux derived from observations of near Earth objects. The impact chronology from these spherule layers reveals that the impactor flux was significantly higher ~3.5 Gyr ago than it is currently. This conclusion is consistent with a gradual decline of the post Late Heavy Bombardment impactor flux.

In chapter 5 (Reprinted from Icarus, Volume 228, B. C. Johnson and H. J. Melosh, Formation of melt droplets, melt fragments, and accretionary impact lapilli during a hypervelocity impact, 347-363, Copyright (2014), with permission from Elsevier.) we focus on material ejected as part of the ejecta curtain and present a model that describes the formation of melt droplets, melt fragments, and accretionary impact lapilli during a hypervelocity impact. Using the iSALE hydrocode, coupled to the ANEOS equation of state for silica, we create high-resolution two-dimensional impact models to track the motion of impact ejecta. We then estimate the size of the ejecta products using simple analytical expressions and information derived from our hydrocode models. Ultimately, our model makes predictions of how the size of the ejecta products depends on impactor size, impact velocity, and ejection velocity. In general, we find that larger impactor sizes result in larger ejecta products and higher ejection velocities result in smaller ejecta product sizes. We find that a 10 km diameter impactor striking at a velocity of 20 km/s creates millimeter scale melt droplets comparable to the melt droplets found in the Chicxulub ejecta curtain layer. Our model also predicts that melt droplets, melt fragments,
and accretionary impact lapilli should be found together in well preserved ejecta curtain layers and that all three ejecta products can form even on airless bodies that lack significant volatile content. This prediction agrees with observations of ejecta from the Sudbury and Chicxulub impacts as well as the presence of accretionary impact lapilli in lunar breccia.

Each of the chapters in this dissertation is meant to stand alone. This is done somewhat out of necessity, because Chapters 4 through 6 represent published papers. This results in some introductory material being repeated, but allows the reader to choose which chapters they wish to read without any ill effects. My advisor Jay Melosh is the sole co-author of the papers that Chapters 4 through 6 represent and by extension he has contributed substantially to the work presented here.
CHAPTER 2. DISTAL IMPACT EJECTA

During the formation of an impact crater, some material is ejected at high velocity. Although there is not a clear definition for distal impact ejecta, we use the definition put forward by Glass and Simonson (2012), that distal impact ejecta is material thrown more than ~2.5 crater diameters from the point of impact. It is difficult to determine exactly when the first distal impact ejecta was recognized (by 29,000 B.C. Humans had found and, evidently, revered tektites) but an impact origin for tektites was not suggested until 1933 (O’Keefe 1976, Spencer 1933).

2.1 Tektites

“… few topics have been characterized by such disagreement and acrimonious debate in the scientific community as the origin of a group of curious, natural glassy objects called tektites” (King 1977).

Coined by Seuss in 1900 from the Greek word for molten, τηκτός, tektites are cm scale previously molten glassy particles (O’keefe 1976). Many tektites have tear-drop or dumbbell shapes indicating they were rotating molten objects (Elkins-Tanton et al. 2003). Some tektites are “button” shaped indicating that ablation took place at some time before they were emplaced (King 1977). The first known written record of tektites is from 950
A.D. (O’keefe 1976). However, Pre-historic humans fashioned simple tools from tektites in Libya around 10,000-20,000 B.C. (Oakley 1952) and a few tektite fragments were found in Willendorf Austria interred in red ochre along with the famous Venus of Willendorf statue, which dates to 29,000 B.C. (O’Keefe 1976). After 500 B.C. tektites were even carried as amulets (O’keefe 1976). It is clear that humans have been interested in these enigmatic particles well before you or me.

Tektites were once thought to be volcanic in origin. They do resemble volcanic glass (except for their low than water content), but they are chemically more similar to sedimentary rocks (Koeberl 1986). Berwerth first noted this chemical similarity in 1917 (King 1977). Suess noted in 1900 that, unlike volcanic glass, tektites are always found loose as individual particles (O’keefe 1976). Armed with these constraints, researchers came up with many hypotheses for the origin of tektites. These ideas included tektites being glassy meteorites, man-made glass distributed by an ancient civilization, ejecta from lunar volcanoes, the products of meteorite ablation, material melted by lightning, material melted by anti-matter falling on the Earth, lunar impact ejecta, and terrestrial impact ejecta (O’keefe 1976, King 1977, and references therein).

By the time the Apollo astronauts returned lunar samples to Earth, most of these tektite formation theories had been refuted. This left lunar impact ejecta, terrestrial impact ejecta, and ejecta from lunar volcanoes as the three major theories for the origin of tektites. The similarities between tektites and glassy particles found around the Wabar and Henbury craters, in Saudi Arabia and Australia respectively, lead Spencer (1933) to hypothesize
that tektites were products of terrestrial impacts. This hypothesis was further supported by the chemical similarity between tektites and terrestrial sediments. With the understanding of glasses at the time, researchers were unable to explain the low water content and relatively reduced iron in tektites. Indeed, lunar samples had low water content and a similar oxidization state to tektites (O’keefe 1970). Other than these similarities, tektites are more like terrestrial sediments than lunar rocks (King et al. 1970, Urey and O’Keefe 1971). Although there were a few staunch defenders of the lunar origin theory, the analysis of lunar samples convinced most researchers that tektites did indeed have a terrestrial origin (King 1977, Koeberl 1986).

Later studies of the noble gas content of tektites show that tektites solidified in the Earth’s atmosphere, further supporting the theory of a terrestrial origin (Matsuda et al. 1993). The noble gas studies also showed that tektites must have solidified high in the atmosphere at altitudes above 20-40 km or pressures below 0.01-0.1 atm (Matsuda et al. 1993). Although the terrestrial impact origin of tektites is generally accepted, the precise mechanism of tektite formation is still debated. Tektites if ejected into the Earth’s ambient atmosphere at the high velocities, implied by the distance that they are found from the source crater, should break up into a fine mist.

One theory suggested to explain the large size of tektites is the idea that tektites are formed from material jetted by an impact (de Gasparis et al. 1975). Jetting occurs early in the impact process, before the projectile is halfway buried in the target. Jetted material is highly shocked and ejected at high velocities, which may exceed the impact velocity
(Vickery 1993). de Gasparis et al. (1975) suggested that analogous to jets’ ability to penetrate deep into solid material, these jets may also penetrate the atmosphere before they break up, allowing tektites to retain their large sizes. However, both experimental and theoretical studies suggest that jetted material should be composed of a mixture of both projectile and target material (Vickery 1993, Miller 1997). This is problematic for the hypothesis that tektites are formed from jetted material because tektites do not exhibit any sign of contamination by projectile material (Koeberl 1986). Thus, it seems more likely that the interaction of the vapor plume and ejecta curtain with the atmosphere are more likely to explain the large size of tektites (Vickery 1993).

The largest known tektite strewn-field is the Australasian field, which has an area of $5 \times 10^7$ km (Simonson and Glass 2004). The true extent of the tektite strewn-fields was not recognized until microtektites were discovered in ocean sediments. In 1967 Glass found that the strewn-fields are actually dominated by microtektites, which are sub-millimeter to millimeter scale previously molten glassy particles that can be spherical, teardrop, or dumbbell shaped (Glass 1967). As I discuss below, tektite-strewn fields are distal impact ejecta layers with some specific properties (Glass and Simonson 2012).

Most ejecta layers contain previously glassy material, which has since become devitrified (crystalized). As their name implies, most impact ejecta layers are found in layer in the stratigraphic record. However, tektite strewn-fields are composed of tektites and microtektites that are still glassy and are often found loose, at least on the continental
crust. These differences are explained by the fact that tektite strewn-fields represent the youngest ejecta layers, with ages less than <35 Myr (Simonson and Glass 2004).

### 2.2 K-Pg Boundary Layer

I now focus on the 66.0 Myr old K-Pg (Properly denominated the Cretaceous-Paleogene, formerly called the K-T or Cretaceous-Tertiary) boundary layer (Renne et al 2013). Although other distal ejecta layers were found before the K-Pg boundary layer, the K-Pg boundary is the most studied ejecta layer and offers the best understanding of how distal ejecta layers form. Additionally, study of this layer has yielded several methods for determining whether a layer has an impact origin. In the next section, I will discuss these other layers.

The K-Pg boundary marks one of the most devastating extinctions in Earth’s history and the end of the dinosaurs’ reign (Alroy 2008, Sheehan and Fastovsky 1992). Globally, the abrupt transition from fossil rich Cretaceous sediments to the fossil poor Paleogene sediments is marked by an ~3 mm thick clay boundary layer (Smit 1999). In 1980, Alvarez et al. found that the boundary layer has a significant iridium anomaly, which they attributed to the impact of a roughly 10 km diameter asteroid. Their work represents the first evidence that the K-Pg boundary layer is an impact ejecta layer.

The original goal of Alvarez et al. (1980) was to estimate the sedimentation rate during the End-Cretaceous extinction. The Earth’s crust and mantle are depleted in Platinum
Group Elements (PGEs), ruthenium, rhodium, palladium, osmium, iridium, and platinum. This depletion occurred early in the Earth’s history during differentiation when the PGEs, which are siderophile (“Iron-loving”) elements, partitioned into the metals that ultimately made up the Earth’s core. Because the Earth is constantly accreting cosmic dust enriched in PGEs, a measurement of the PGE concentration in a sedimentary rock allows one to estimate the sedimentation rate (Barker and Anders 1968).

Alvarez et al. (1980) showed that the iridium concentration of the boundary layer in Italy, Denmark, and New Zealand, was respectively 30, 160, and 20 times the background concentration. They also found that the sedimentation rate at all three sites was nearly the same above and below the boundary clay. Thus, Alvarez et al. (1980) attributed the Iridium anomaly to a large influx of extraterrestrial material rather than a large drop in the sedimentation rate. Then, using the known iridium concentration of a carbonaceous chondrite, (carbonaceous chondrites are considered to be typical composition of solar system solids) and assuming that the layer is globally uniform, they estimated that the layer was created by the impact of a 10 ± 4 km diameter object.

In addition to the enrichment in PGEs found in 1980, the discovery of shocked quartz (Bohor et al. 1984); impact spherules (Smit and Klaver 1981) containing nickel rich spinel (Montanari et al 1983, Kyte and Smit 1986); and chromium isotope data consistent with an extraterrestrial source (Shukolykov and Lugmair 1998) have all strengthened the hypothesis that the K-Pg boundary layer was created in the aftermath of an
extraterrestrial impact. I will describe each of the methods to determine an impact or extraterrestrial origin in more detail in section 2.4.

Once an impact origin for the K-Pg boundary was suggested, a concerted effort to find additional K-Pg boundary sites and a potential source crater began. Although several craters with ages around 66 Myr were known, none of them were large enough to explain the observed layer (Grieve 1987). The originally basaltic composition of spherules within the layer seemed to indicate an impact into oceanic crust (Montanari et al. 1983) while the presence of shocked quartz grains in the layer implied an impact into continental crust (Bohor et al. 1984). Jones and Kodis (1982) argued that the ~3mm thick global layer was ejected ballistically as part of a rapidly expanding fireball composed of projectile and target material vaporized by the impact. Colgate and Petschek (1985) argued that the ballistic ejection of vaporized material was limited to distances of ~400 km from the source crater and that this hot material subsequently floated on top of the atmosphere before being deposited as the global K-Pg boundary layer. However, this floating ejecta scenario does not explain the observed two layer structure found up to ~5000 km from the impact site or how global wild fires might have started (Schulte et al. 2010, Robertson et al. 2013, Melosh et al. 1990, Goldin and Melosh 2009).

Bohor et al. (1987) realized that at a rather well preserved site in Wyoming, the K-Pg boundary has a two-layer structure. Here, the typical 3 mm iridium rich spherule layer lies atop an ~3 cm thick spherule layer that does not have a significant iridium anomaly. This thicker layer is attributed to less energetic ejecta restricted to a region closer to the
point of impact (Hildebrand and Boynton 1990, Smit and Romein 1985). Thus, a site with a thicker boundary layer is assumed to be closer to the source crater (Hildebrand and Boynton 1990).

The discovery of ~50 cm thick K-Pg boundary deposit in Haiti and “impact wave” or tsunami deposits in the Caribbean, along with a plate tectonic reconstruction of the area ~65 Myr ago, lead Hildebrand and Boynton (1990) to conclude that the K-Pg impact occurred somewhere between North and South America. In 1991, Hildebrand et al. took note of gravity and magnetic anomalies near the northwestern margin of the Yucatan peninsula of Mexico. In 1975, Ramos attributed these geophysical anomalies to a volcanic complex, but in 1981, Penfield and Camargo attributed them to an impact crater (Hildebrand et al. 1991). Hildebrand et al. (1991) also found that these anomalies were consistent with a roughly ~200 km diameter impact structure which they dubbed the Chicxulub crater. The stratigraphy of core samples from nearby oil wells showed that this new impact structure had an age similar to the K-Pg boundary (Hildebrand et al. 1991).

Since 1980, the K-Pg boundary has been studied at over 350 unique sites (Schulte et al. 2010). These sites show that a roughly 3 mm thick layer composed of closely packed 250 micron diameter spherules covers the entire Earth (Smit 1999). This layer, which formed as the result of the fast expansion of a massive plume of material vaporized by the impact, contains the extraterrestrial signature of the impactor. Sites within ~5000 km of the Chicxulub crater have a thicker secondary layer that underlies the global fireball layer (Schulte et al. 2010). The thickness of this layer increases from a few cm to over 100 m
thick at the rim of the Chicxulub crater. This layer contains impact spherules, solid ejecta, and particles that look similar to volcanic accretionary lapilli (Schulte et al. 2010). This decrease in thickness with distance from the source crater is consistent with material ejected as part of the excavation flow during the formation of the crater.

Although the link between the end Cretaceous extinction and the Chicxulub impact are generally accepted (Schulte 2010), the kill mechanisms responsible for the extinction are actively debated. Because the end Cretaceous extinction occurred globally, many of the suggested kill mechanism involve material ejected by the impact in some capacity. Some of these mechanisms include thermal radiation emitted by high speed ejecta re-entering the atmosphere (Melosh et al. 1990, Goldin and Melosh 2009), which may have even started global wild fires (Robertson et al. 2013); ocean acidification caused by sulfuric acid originating from SO$_2$ volatized from target rock (D’Hondt et al. 1994); ocean acidification caused by Nitric acid from NO$_x$ created by high velocity ejecta heating the atmosphere (Prinn and Fegley 1987); and impact winter (Alvarez et al. 1980). Geologic evidence seems to favor the global wild fire and ocean acidification mechanisms (Robertson et al. 2013, Alegret et al. 2012).

All of the above kill mechanisms depend on the details of impact ejection and re-entry into our atmosphere. Understanding which kill mechanisms are responsible for the mass-extinction, their extent and duration can help us understand how the biosphere reacts to such a catastrophe and may have implications for early life on earth when the bombardment rate was thought to be significantly higher than it is today (Bottke et al.
2012). It is clear that understanding the dynamics of the formation, ejection, and atmospheric re-entry of distal impact ejecta is of great importance.

2.3 Other Ejecta Layers

Prior to 1980 and the discovery that the K-Pg boundary layer is an impact ejecta layer, only five distal impact ejecta layers were known (Glass and Simonson 2013). Currently there are 26 known distal ejecta layers but only eight layers have been associated with a source crater (Glass and Simonson 2013). The steady increase of the number of recognized layers over the past three decades implies that many more distal ejecta layers are yet to be found. The currently recognized layers range in age from ~0.8-3470 Myr old (Glass and Simonson 2012). Typically, these layers are composed of sub-millimeter to millimeter size previously molten spherules (Simonson and Glass 2004). Some of these layers are composed of closely packed spherules and are up to 10’s of centimeters thick while other layers are sparse having an average thickness less than the size of a single spherule (Glass and Simonson 2012).

2.3.1 Evidence to support an impact origin

In addition to an anomalous concentration of Ir and other PGEs there are several other observations that indicate an impact origin of an ejecta layer.
2.3.1.1 **Impact Spherules**

The easiest way to identify a distal impact ejecta layer it to find previously molten spherules. Although a glassy spherule would indicate it was previously molten, some spherules crystalized as they cooled (Smit and Klaver 1981, Montanari et al. 1983). Additionally, some spherules that were originally glassy have been almost completely replaced by secondary minerals and/or devitrified, meaning the original glass has crystalized (Simonson and Glass 2004). One method to determine that the spherule were previously molten is to find one or more vesicles within the spherule (Glass and Simonson 2012). Rare spherules with rotational forms, shaped like dumbbells or teardrops, also indicate that the spherules were once molten (Simonson and Glass 2004). The presence of previously molten spherules does not necessarily imply an impact origin as previously molten spherules can also have a volcanic origin. However, ash will accompany volcanic spherules and volcanic deposits will be restricted to a smaller geographical area than impact spherules (Glass and Simonson 2012).

As previously mentioned, some spherules contain Nickel rich spinel, which has a composition that is unlike any terrestrial spinel (Kyte and Smit 1986). Robin et al (1992) showed that Ni-rich spinel found in impact spherules is similar in composition and oxidization state to the relatively oxidized spinel found in the fusion crusts of meteorites (fusion crust is a thin glassy coating that forms as by melting and ablation of meteorites during their entry into the Earth’s atmosphere). Ni-rich spinel found in impact spherules likely forms in the oxidizing condition of the impact vapor plume (Ebel and Grossmann...
2005). Ni-rich spinel seems to be resistant to weathering and mineral replacement as indicated by the preservation of Ni-rich spinel in 3.5 Gyr old Archean spherules (Byerly and Lowe 1994).

2.3.1.2 Isotopic Data

Although an extraterrestrial source might explain the increased Ir and other PGEs in the K-Pg boundary, Hallam (1987) argued that volcanism could also explain the Ir anomaly. Indeed, lavas sourced from the deep mantle exhibit significant Ir enrichment when compared to crustal rocks (Hallam 1987). However, hydrothermal processes or the inclusion of ultramafic rocks only produce Ir enrichments as high as a few hundred parts per trillion (French and Koeberl 2010). For reference K-Pg boundary has an Ir enrichment of a few to tens of parts per billion (Alvarez et al. 1980, Shculte et al. 2010). Regardless, as previously mentioned, Cr isotopic data shows that the K-Pg boundary has an extraterrestrial origin (Shukolyukov and Lugmair 1998). Furthermore, the inter element ratios of PGEs of meteorites differ significantly from terrestrial rocks (Koeberl et al. 2012).

The Chromium isotope method developed by Shukolyukov and Lugmair (1998) is arguably the most robust way to determine the extraterrestrial origin of an ejecta layer (Koeberl et al. 2012). $^{53}$Cr is the stable product of the decay of $^{53}$Mn, which has a half-life of 3.7 Myr. Because the Earth differentiated long after the decay of $^{53}$Mn, terrestrial rocks show no variation in $^{53}$Cr/$^{52}$Cr (Koeberl et al. 2012). The ratio of $^{53}$Cr/$^{52}$Cr is a
measure of how much $^{53}$Mn was present when a solar system body formed. All known meteorite groups differ from the Earth’s $^{53}$Cr/$^{52}$Cr ratio (Shukolyukov and Lugmair 1998). Additionally, because meteorites typically have a much higher Cr abundance than the Earth’s crust, a small addition of extraterrestrial material can dominate the Cr observed in an ejecta layer (Shukolyukov and Lugmair 1998).

The $^{53}$Cr/$^{52}$Cr ratio of the K-Pg boundary layer is consistent with the layer containing carbonaceous chondrite material (Shukolyukov and Lugmair 1998). In the same year, Kyte (1998) found a 2.5 mm fossilized meteorite in the K-Pg boundary layer. This fragment is geochemically similar to a carbonaceous chondrite, and Kyte (1998) concluded that the fragment was a surviving piece of the extraterrestrial object that created the Chicxulub crater and the K-Pg boundary layer. The extraterrestrial origin of six other spherule layers has been determined using Chromium isotopes (Glass and Simonson 2012).

In addition to Cr isotopes, Os isotopes also suggest an extra terrestrial origin for ejecta layer. However, mantle rocks have a similar $^{187}$Os/$^{188}$Os ratio to meteorites. Thus, one could argue that Os isotope anomalies are the product of volcanism if the lavas contain mantle material. However, the inter element ratios of PGEs of meteorites differ significantly from terrestrial rocks (Koeberl et al. 2012). For a brief introduction to other proposed geochemical indicators of an impact or extraterrestrial origin, see Koeberl et al. (2012).
The signature of an extraterrestrial component of a layer surely implies that it has an impact origin. However, the lower layer of the Chicxulub ejecta, which is composed of less energetic material ejected as part of the ejecta curtain, shows no evidence of extraterrestrial contamination (Schulte et al. 2010). Similarly, tektites and the tektite-strewn fields show no sign of a meteoritic component. Thus, an extraterrestrial signature cannot be required to identify a layer’s impact origin.

2.3.1.3 Shocked Quartz

The presence of shocked quartz is arguably the strongest indicator that an ejecta layer was created by an impact. Additionally, shocked quartz can act as a shock barometer, indicating the peak shock pressures that material reached. Quartz grains that are lightly shocked to $<10$ GPa exhibit planar fractures (Langenhorst and Deutsch 2012). Planar Deformation Features (PDFs), which are submicron thick amorphous lamalae, are produced when quartz is shocked to pressures between 10 and 30 GPa (French and Koeberl 2010). These features are especially indicative of impact, because no other known natural processes are capable of creating the high strain rates and pressures required to make these features (French and Koeberl 2010).

Coesite or stishovite, two high-pressure polymorphs of silica that crystalize from shock-melted quartz during release from high pressure, may also indicate formation by an impact (French and Koeberl 2010, Langenhorst and Deutsch 2012). In addition to coesite
and stishovite, high-pressure polymorphs of many other minerals are used as indicators of the high shock pressure produced by impacts (Langenhorst and Deutsch 2012).

\subsection{Ejecta Layers as Record of Impacts}

Impact ejecta layers cover an area much larger than their source crater and for a large enough impact may blanket the entire globe (Schulte et al. 2010). Because impacts represent geologically instantaneous events, these ejecta layers act as excellent markers of time in the stratigraphic record (Simonson and Glass 2004). As previously mentioned, there are currently 26 recognized distal ejecta layers (Glass and Simonson 2013). However, only eight layers have been associated with a source crater (Glass and Simonson 2013) and we do not expect that many other source craters will be found.

The Earth’s crust is \( \sim 70\% \) oceanic crust by area. Because oceanic crust is constantly being recycled, the oldest oceanic crust is \( \sim 280 \) Myr old while the average age of oceanic crust is closer to \( 65 \) Myr old (Müller et al. 2008). Thus, we expect that only \( \sim 30\% \) of impacts craters older than 280 Myr will be observable today. Additionally, we know that the continental crust is less than \( \sim 2 \) Gyr old on average (Allègre and Rousseau 1984, Hawkesworth and Kemp 2006). Because only 15\% of the Earth’s crust is older than \( \sim 2 \) Gyr (eg. half of the Earth’s continental crust), we expect that only \( \sim 15\% \) of craters older than \( \sim 2 \) Gyr will survive until the present time. These estimates are somewhat generous, as they neglect weathering, burial, and other tectonic effects that may obscure or destroy
a crater. Neglecting these other effects, Figure 2.1 shows an estimate for the probability that a crater of a given age will survive until today.

![Figure 2.1 Probability of Crater Survival on Earth](image)

The probability that a crater will survive to present day is plotted as a function of when the impact occurs. The probability is calculated as equal to the fraction of the Earth’s crust that is of a given age (Müller et al. 2008, Allègre and Rousseau 1984, Hawkesworth and Kemp 2006). Thus, the probability assumes that any given impact will strike a random point on the Earth.

Both Popigai and Manicouagan are larger than ~85 km in diameter and have been associated with global spherule layers (Glass and Simonson 2012, Onoue et al. 2012). Thus, we assume that any impact capable of creating a crater larger than 85 km in
diameter will also create a global spherule layer. To estimate the size of an impactor needed to create a crater larger than 85 km, crater scaling becomes necessary. Assuming that the impactor and target have similar densities, the transient crater diameter, which is the diameter of a crater before it begins to collapse, is given by the following equation from Melosh (2011)

\[ D_t = 1.161 \ D_{imp}^{0.78} \ v_{imp}^{0.44} \ g^{-0.22} \ \sin^{1/3}(\theta) \]  

(SI units)

where \( D_{imp} \) is the impactor diameter; \( v_{imp} \) is the impact velocity assumed to be 20 km/s the typical velocity for asteroids striking the Earth (Minton and Malhotra 2010); \( g \) is the surface gravity of Earth; and \( \theta \) is the impact angle, which is assumed to be the average of 45 degrees. On Earth, a crater with a diameter larger than \( D_{s-c}=3.2 \) km will collapse to form a complex crater. The final size of a complex crater is related to the transient crater diameter by the following equation from Melosh (2011)

\[ D = 1.17 \ D_{imp}^{1.3} \ D_{s-c}^{-1.3} \]

Using these two equations, we find that a roughly 7.4 km diameter impactor is required to create a 85 km diameter crater on Earth for typical impact condition of \( v_{imp} = 20 \) km/s and \( \theta = 45 \) degrees. According to observation of near earth objects, the probability that an impactor larger than 7.4 km in diameter will hit the Earth is \( \sim 1.4 \times 10^{-8} /\text{yr} \) (Stuart and Binzel 2004). The impact chronology of the Moon implies that the impactor flux has remained relatively constant for the past 3 Gyr (Neukum et al. 2001). However, dynamical models estimate that the impactor flux was two times higher \( \sim 2-3 \) Gyr ago (Minton and Malhotra 2010, Durda et al. 1998).
Figure 2.2 shows the estimated number of craters younger than a given age produced on Earth assuming both a constant impactor flux and an impactor flux that steadily increases as we go back in time (Minton and Malhotra 2010). The figure shows that for a constant impactor flux we expect there should have been \(~49 \pm 7\) impacts that can create global spherule layers in the past 3.5 Gyr. While the impactor flux of Minton and Malhotra (2010) implies that there should have been \(~113 \pm 11\) in the same period.

![Figure 2.2 Total Number of Craters Larger than 85 km in Diameter on Earth](image)

The black dashed line is the total number of craters younger than a given age that should have produced 85 km diameter or large craters on Earth assuming a constant impactor flux of \(1.4 \times 10^{-8}\) /yr. The dashed blue curve assumes the constantly decreasing impactor flux estimated by Minton and Malhotra (2010). The flux rate from Minton and Malhotra (2010) is normalized so that the current day flux is \(1.4 \times 10^{-8}\) /yr. The error bars plotted at 0.5 Gyr intervals assume poisson statistics (ie. \(\sqrt{N}\)).

By combining the cumulative number of impacts from Figure 2.2 with the probability of crater survival from Figure 2.1, we can estimate how many craters with diameters larger than 85 km should still exist on Earth’s crust today. Assuming that the impactor flux has been constant throughout Earth’s history, we find that \(~8 \pm 3\) craters larger than 85 km in
diameter should have formed during the past 3.5 Gyr, and survived until today (Figure 2.3). While the steadily decreasing impactor flux predicted by Minton and Malhotra (2010) produces \(~11 \pm 3\) surviving craters during the same interval. Even though the steadily decreasing flux produces more than two times the number of craters a constant flux does, the number of surviving craters each model produces are within the 1-\(\sigma\) uncertainty of each other. This illustrates how insensitive the cratering record on Earth is to past changes in the impactor flux. This is because most of the ancient rocks have been removed or recycled creating a strong bias toward younger ages. The fact that we have found 6 craters larger than 85 km in diameter while we expect to have \(8 \pm 3\) based on our quite conservative calculation, indicates that we have probably found most, if not all of the large craters that still remain on Earth.

Assuming a constant impactor flux over the past 3.5 Gyr, we expect that \(~49\) impacts large enough to create global spherule layers should have occurred. This means that the only indication of \(~85\%\) of large impacts over the past 3.5 Gyr are the spherule layers they leave behind. The fraction of surviving craters to expected craters only becomes smaller if you assume that the impactor flux was higher in the past than it is today. Thus, we argue that the search for spherule layers in the stratigraphic record is much more likely to be fruitful than searches for large impact craters. Although we expect many more spherule layers to be found, it is important to note that spherule layers may be difficult or impossible to find in highly metamorphosed rocks (Simonson and Glass 2004).
Because impact craters are quickly destroyed or obscured on Earth, the Earth’s impact history is usually inferred from the uncertain impact chronology of the Moon or estimates of the current day impactor flux (Neukum et al. 2001, Stuart and Binzel 2004). The Moon’s cratering record indicates that there may have been a large increase in impactor flux ~600 Myr after the solar systems formation from 4.0-3.7 Gyr ago, called the Late Heavy Bombardment (LHB). One explanation for the LHB is the Nice model (named after Nice France where the model was conceived) (Gomes et al 2005). In this dynamical model the slow outward migration of gas-giant planets changes abruptly when Saturn and Jupiter cross a 2:1 mean motion resonance. This rapid change causes many orbits to become unstable, sending numerous impactors in toward the Earth and the Moon. A further addition of the Nice model, which includes an extension of the asteroid belt or so called “E-belt”, predicts a slow decrease in the post LHB impactor flux (Bottke et al. 2012).

Estimates of the magnitude and duration of LHB based on the Moon’s cratering record have large uncertainties (Fasset and Minton 2013). Without more lunar samples, constrains on the LHB based on the lunar record are unlikely to become more rigid. However, if spherule layers can be used to estimate sizes of the bodies that created them, spherule layers may provide estimates of the Earth’s bombardment history. This bombardment history would provide important constraints for models of the early solar system and its evolution. Additionally, a better understanding of the Earth’s bombardment history also has implications for life. As previously discussed, impacts can have devastating consequences for life. However, impacts have also been proposed as a
source of hydro thermal systems, amino acids, and reduced phosphorous that are essential to early life (Cockell 2006, Pierazzo and Chyba 1999, Pasek et al. 2013). It is clear that understanding how distal ejecta layers form is of great importance.

Figure 2.3 Number of Surviving Craters Larger Than 85 km in Diameter on Earth

The solid black curve is the total number of craters younger than a given age that we expect should have survived until current day assuming a constant impactor flux of $1.4 \times 10^{-8} \text{/yr}$. We create this curve by integrating the product of probability shown in Figure 2.1 and the constant impactor flux of $1.4 \times 10^{-8} \text{/yr}$ through time. The solid blue curve is the total number of craters younger than a given age that we expect should have survived until current day assuming a steadily decreasing flux (Minton and Malhotra 2010). We create this curve by integrating the product of probability shown in Figure 2.1 and the flux from Minton and Malhotra (2010) through time. The points on the solid blue and black curves are at integer values and the associated error bars are calculated assuming Poisson statistics (ie. $\sqrt{N}$). The red curve and the points on it represent the observed cumulative number of impacts younger than a given age based on Table 2.1.
Table 2.1 Craters Larger than 85 km in Diameter

The crater sizes and ages reported in this table are from the Earth Impact Database (http://www.pasc.net/EarthImpactDatabase/). Although Popigai and Manicouagan have been estimated to be 100 km in diameter, the size estimates from the Earth Impact Database ideally represent the consensus of the scientific community. The next largest crater is the 70 km diameter Morokweng crater. The associated spherule layers are from Glass and Simonson (2012) and references therein, except for the Karelian layer, which is from (Huber et al. 2012).

<table>
<thead>
<tr>
<th>Crater Name</th>
<th>Age (Myr)</th>
<th>Size (km)</th>
<th>Spherule Layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Popigai</td>
<td>35.7</td>
<td>90</td>
<td>Cpx spherule</td>
</tr>
<tr>
<td>Chicxulub</td>
<td>65</td>
<td>150</td>
<td>K-Pg Boundary</td>
</tr>
<tr>
<td>Manicouagan</td>
<td>214</td>
<td>85</td>
<td>Late Triassic spherule</td>
</tr>
<tr>
<td>Acraman</td>
<td>~590</td>
<td>90</td>
<td>Acraman</td>
</tr>
<tr>
<td>Sudbury</td>
<td>1850</td>
<td>130</td>
<td>Sudbury</td>
</tr>
<tr>
<td>Vredefort</td>
<td>2023</td>
<td>160</td>
<td>Karelian</td>
</tr>
</tbody>
</table>
CHAPTER 3. FORMATION OF SPHERULES IN IMPACT PRODUCED VAPOR PLUMES


We have constructed a numerical model of spherule formation in an impact produced vapor plume. This model tracks the expansion of the vapor plume using a one-dimensional Lagrangian hydrocode coupled with the ANEOS equation of state for silica. We then include the equations for nucleation and growth as described by homogeneous nucleation theory to describe the process of spherule formation. We use this model to determine the number and size of the spherules that an impact creates. We also explore when and where spherules are formed in the vapor plume, and how this affects the size of the spherules. In general we find that smaller spherules form in the outer, faster moving, portions of the vapor plume at earlier times. This work also explores the effect of impactor size and impact velocity on the resultant spherule size. We report a simple linear dependence on impactor size and a complex dependence on impact velocity. We find that a 10 km diameter asteroid impacting at a velocity of ~21 km/s creates spherules that are ~250 μm in diameter which is comparable to the spherules found in the K/Pg boundary layer.
3.1 Introduction

The “smoking gun” that first demonstrated that the Cretaceous era was ended by a large asteroid impact was a thin but global layer of ejecta (Alvarez et al 1980). Containing elevated levels of iridium and packed with 250 mm spherules, the terminal K/Pg layer is typically about 3 mm thick and, at the best preserved locations, is composed of spherules in a clay matrix whose volume is roughly equal to that of the spherules themselves (Smit, 1999). The spherules, currently composed mainly of the mineral sanidine, probably originated as a mafic glass consisting of a mixture of projectile and target materials. This glass recrystallized shortly after deposition and weathered to its present form.

Other ancient impacts have been similarly recognized from their globally distributed ejecta deposits. In almost all cases, these distal ejecta contain spherules that originated as glassy droplets ejected from the impact crater at high speed (Simonson and Glass, 2004). Such spherule layers are often our best (and may be our only) indication of the existence of an ancient impact. It is therefore of great importance to understand how such spherules form and to find some means to relate the properties of the observed spherule deposits to the size and nature of the impact that created them.

The overall mechanics of impact cratering are now reasonably well understood (Melosh, 1989). When an asteroid or comet strikes the Earth at high speed its kinetic energy is converted to heat and motion of both the impactor itself and of the target material. The kinetic energy of the impactor is initially confined to a volume comparable to that of the
impactor itself. As the cratering process unfolds, this energy is transferred to the target and diluted as more material is engulfed by an expanding shock wave. The ultimate result is a crater whose diameter is typically 10 or 20 times larger than the original projectile. The most distal deposits, however, are formed by ejecta launched early in the cratering process when energy densities are high enough to expel material at velocities comparable to the impact velocity.

Numerical studies of the early stages of high-speed impacts have long shown that the highest pressures and internal energies are localized in an approximately uniform “isobaric core” comparable in size to the projectile (Pierazzo et al 1997). This volume is comprised of both projectile and target material. At impact velocities greater than about 16 km/sec the internal energy deposited in this region is large enough to vaporize this material, which expands rapidly away from the impact site. The vapor initially forms a hot, high-pressure supercritical gas that expands in an approximately adiabatic fashion into open space above the impact site. Less highly shocked material follows this early, fast, vapor expansion to form the ejecta curtain familiar from low velocity impact experiments. While the slower ejecta curtain is deposited near the point of impact (typically most of this material falls within one diameter of the final crater), the high velocity ejecta create the distal layer of spherules.

In this paper, we argue that the spherules that form a global ejecta layer condensed from rock vaporized by the impact. Other melt spherules, less widely distributed, originated from less highly shocked target rocks and lack the distinctive chemical and isotopic
signatures of admixture with the projectile. These two spherule origins are distinguished by their thermodynamic histories: the most energetic spherules condense from vapor and their thermodynamic history begins at a shock state on the Hugoniot curve, then follows an adiabat that intersects the melt-vapor coexistence curve from the vapor side (Figure 3.1). These spherules are the subject of this paper. Less shocked material (mostly originating from the target rocks) follows a thermodynamic path that intersects the coexistence curve from the liquid side. We name spherules formed in this way melt droplets. Melt droplets form when the expanding supercritical fluid boils upon reaching the coexistence curve (Melosh and Vickery, 1991).

To avoid confusion, we make the distinction between vapor-condensed spherules and melt droplets precise. The dividing line between the two is the shock release curve that leads from a Hugoniot shock state to the critical point on the phase curve of the material that composes the projectile-target mixture in the isobaric core of the impact. For example, using the well-defined ANEOS equation of state for SiO\textsubscript{2} at high pressure (Melosh 2007), and starting at fully dense quartz at standard temperature and pressure, this is the shock state at a pressure of 315 GPa, temperature of 21,100 K and particle velocity of 8.2 km/sec. It corresponds to an impact of quartz-on-quartz at a velocity of 16.3 km/sec. In the discussion we argue that more realistic projectile and target compositions than quartz will yield similar conditions.
Figure 3.1 Release Adiabats

Thermodynamic paths of the adiabatic release of shocked SiO2 from high pressure on a log P versus T diagram. The Hugoniot curve, indicating the final result of increasingly strong shock compression of quartz, is shown as a heavy line, while the thin colored lines are decompression adiabats. The liquid/vapor coexistence curve separating liquid and solid phases is shown as a heavy line and the critical point by a heavy dot. The numbers labeling the release adiabats are the particle velocities in the shocked material in km/s. These velocities can be interpreted as the outcome of an impact experiment between identical materials at twice the particle velocity. Thus, the curve labeled 7 is the release adiabat of a face-on impact between two quartz plates at 14 km/s. Material described by the blue adiabats decompresses and forms a boiling liquid when it reaches the phase curve creating melt droplets. The red adiabats are so strongly shocked that they decompress forming vapor that then condenses into spherules when the adiabat reaches the coexistence curve.

In this paper we focus upon the nucleation and growth of spherules in a hot, freely expanding silicate vapor plume. Although most asteroids are mafic in composition, being
mainly composed of a combination of about 50% silica (by mass) along with the oxides of magnesium and iron, we focus on the condensation of pure silica vapor because of the abundance of thermodynamic data for this material. Although we expect that our results will differ in detail from those using more realistic materials, we believe that the major outlines of the condensation process will be similar for all silicate materials. Our analysis also demonstrates which thermodynamic properties are the most important determinants of spherule size.

In accordance with our simplified material model, we also use a simplified impact model to avoid obscuring the major features of the condensation process. Rather than coupling the condensation computation to a full two- or three-dimensional hydrocode computation, we use a simple one-dimensional Lagrangian hydrocode (described in Appendix A.2) that models the hemispherical expansion of an initially uniform half-sphere of highly shocked material representing the essential properties of the isobaric core. In the future, condensation computations of this type may be coupled with more realistic hydrocode simulations, although such coupling will probably be computationally intensive. We believe that our current results are sufficiently robust that they correctly represent the major features of vapor plume condensation, a process that is both highly important and that has not been adequately treated in previous impact studies.

Several previous attempts to describe the process of spherule formation have predicted the K/Pg spherule size within an order of magnitude (de Neim 2002; O'keefe & Ahrens 1982; Melosh & Vickery 1991). When we consider the difference between spherules and
melt droplets, we find the work by Melosh and Vickery applies only to melt droplets and not to spherules or spherule formation. The other two studies are consistent with our definition that describes spherules as vapor condensates using the theory of homogeneous nucleation. Although this work builds on the foundation established in previous works, we feel a new model is necessary to better understand the process of spherule formation.

O'keefe & Ahrens (1982) used the analytical approximations for nucleation and growth of spherules in an expanding vapor plume developed by Raízer (1960). These approximations used the ideal gas equation of state and the average properties of the vapor plume. In addition, O’keefe and Ahrens (1982) approximated the internal energy of the vapor plume as a constant, independent of impact velocity. We argue that the initial internal energy in the vapor plume and the energy in the isobaric core are related. This means the vapor plume has an energy $U \propto u_p^2 \propto V_{imp}^2$, where $u_p$ is the maximum particle velocity, and $V_{imp}$ is the impact velocity (Melosh 1989). O'keefe & Ahrens (1982) also approximated the vaporization energy per unit mass of silicates to be identical to that of iron. Considering the many approximations used in their work, it seems fortuitous that it predicts spherule sizes that agree with observation of the K/Pg boundary layer to a factor of order unity.

de Neim (2002) uses a more realistic Van der Waals equation of state and a two-dimensional model for the expanding vapor plume. He also solves the equations for nucleation and growth numerically rather than relying on approximations. Regardless of these improvements, de Neim’s model predicts spherule sizes that are $\sim$10 times larger
than those observed in the K/Pg boundary layer. Although the model seems capable of extension, de Neim did not explore the spherule sizes created by various impact velocities and impactor sizes. His model should also be capable of determining a spatial dependence of spherule sizes within the vapor plume but no attempt was made. The model by de Neim (2002) calculates multiple generations of spherules. We argue that multiple nucleation events are unphysical on the grounds of kinetic frustration, which we describe in Appendix A.5.

Kinetic nucleation theory, as described in Appendix A.1, gives an expression for the rate at which spherules form. This rate has a strong exponential dependence on the surface energy, making an accurate description of surface energy extremely important. Previous works by O'Keefe and Ahrens, and by de Neim use a constant value for surface energy. We argue that the surface energy should depend on temperature and that it must vanish at the critical temperature. Our work demonstrates the importance of this temperature dependence. In addition to an inaccurate description of the surface energy, the previous works are based on Classical Nucleation Theory described by Becker-Döring (1935) and Zel'dovich (1940). As we describe in Appendix A.1 Classical Nucleation Theory has been replaced by Kinetic Nucleation Theory, which makes fewer assumptions and has a much better agreement with experiment. (Katz and Weidersich 1977, Girshick and Chiu 1990). In this chapter, we put forward a model that includes a more robust equation of state, a more accurate expression for the temperature dependence of surface energy, more accurate equations for nucleation and growth, and the ability to resolve both spatial and temporal aspects of the spherule forming process.
3.2 Methods

The results that come from homogeneous nucleation theory depend on thermodynamic variables on and near the liquid/vapor coexistence curve. For this reason an equation of state that can accurately describe the two-phase system is important. We assume both the impactor and target are made of SiO$_2$ in order to use the ANEOS equation of state for silica (Melsoh 2007). Recent experiments reveal that ANEOS describes the liquid/vapor coexistence curve and critical point well. These same experiments also indicate that the pressure-entropy Hugoniot predicted by ANEOS is accurate (Kraus et al. 2011).

To use a one-dimensional Lagrangian hydrocode to model the expansion of the vapor plume we have to make some major simplifications and assumptions. We treat the vapor plume as a homogeneous hemisphere, which is initially at rest. The hemisphere then expands into free space without the effect of gravity. The acceleration due to gravity will be small when compared to the expansion velocity, which is comparable to the impact velocity. As such, at early times gravity will have little effect on the expanding vapor plume. We assume that the initial vapor plume is composed of material initially contained within the isobaric core, the central most highly shocked region of an impact. By definition, the isobaric core is a region with spatially constant maximum shock pressure. This region is a sphere with radius $R_{ic} \sim R_{proj}$, the radius of the projectile. To be more precise, $\log \left( \frac{R_{ic}}{R_{proj}} \right) = -0.346 + 0.211 \log \left( \frac{V_{imp}}{1 \text{km/s}} \right)$ where $V_{imp}$ is the impact velocity (Pierazzo et al. 1997). Outside of the isobaric core, the shock pressure falls off
approximately as the square of the distance. This motivates the approximation that all vaporized material will be contained in the isobaric core. Because the vapor plume is hemispherical and the isobaric core is spherical we assign an initial radius to the vapor plume of \( r_o = R_{ic} \frac{1}{2}, \) which gives the model vapor plume the same volume as the actual isobaric core.

Because we assume that the impactor and target are made of the same material, the average particle velocity \( u_p \) in the isobaric core is approximately half of the impact velocity (Melosh 1989). Through the Hugoniot calculated by ANEOS, \( u_p \) uniquely defines the density of the isobaric core. These assumptions and simplifications lead to the initial conditions of a homogeneous hemisphere initially at rest with a size, internal energy, and density determined by the size and velocity of the impactor. With these simplified initial conditions, we believe a one-dimensional Lagrangian hydrocode is a robust model. As with any Lagrangian hydrocode, we must partition our system into a number of cells. We find that our model converges when we use 160 equally massive hemispherical cells to resolve the expanding plume.

We use a one-dimensional Lagrangian hydrocode to track the expansion of the vapor plume and include the equations for nucleation and growth to determine the spherule size. Although it is helpful to understand the process of spherule formation, an in-depth knowledge of the model is not necessary to understand the results. For this reason we explain the majority of the model in the various appendices. In Appendix A.1, we
introduce the theory of homogeneous nucleation as well as the equations for growth. In Appendix A.2, we explain our hydrocode model and the numerical methods we use to solve the nucleation and the growth equations. In Appendix A.3, we describe the temperature dependent expression for surface energy. In Appendix A.4, we explain the equilibrium chemistry model that we have included. In Appendix A.5 we explain the process of quenching and introduce the concept of kinetically frustrated nucleation.

3.3 Results

3.3.1 Spherule Formation

The process of spherule formation occurs in four steps. The first step is the adiabatic expansion of the vapor plume. After some adiabatic expansion the vapor comes to the liquid/vapor coexistence curve or phase boundary (Expansion 3.3.2). As the vapor continues to expand and cool, it becomes supercooled. This is when nucleation, the second step, begins; at this time nuclei (large molecular clusters) begin to form releasing latent heat. As the degree of supercooling increases, the nucleation rate (rate that new nuclei are created) increases, as does the rate at which latent heat is released. As the degree of supercooling increases so does the rate at which nuclei grow to supercritical sizes. This also increases the rate at which latent heat is released. When enough latent heat is liberated, the temperature of the two-phase system increases, forcing the adiabat back to the liquid/vapor coexistence curve. At this time, the system is no longer supercooled and nucleation ceases (3.3.3 Nucleation). During the third step, called
growth, vapor condenses onto existing spherules making them grow as the vapor plume continues to expand. As the spherules grow to macroscopic size, latent heat is released and the two-phase system follows the path of the liquid/vapor coexistence curve (Growth and Quenching 3.3.4). The fourth and final step is quenching. Quenching occurs because the growth rate is limited by how often vapor molecules collide with a spherule. As the plume continues to expand and cool, the vapor becomes so sparse that collisions between vapor molecules and spherules become rare. At this point, growth stops and the adiabat leaves the coexistence curve. When growth stops a significant amount of uncondensed vapor is still in the system. Quenching, the fourth and final step, brings spherule growth to a halt (Growth and Quenching 3.3.4). The initial impact and the process of spherule formation are illustrated in Figure 3.2. The figure illustrates where and when the different phases of spherule formation take place, within the vapor plume created by a 10km diameter impactor with an impact velocity of 21 km/s.
Three cartoons that illustrate the initial impact and four phases of nucleation. Figure 3.2.a (top) illustrates a 10 km diameter impactor with an impact velocity of 21 km/s just before impact. Figure 3.2.b (middle) shows the expanding hemispherical vapor plume created by the impact after 1.29 seconds of expansion. The dots, which are not to scale, represent spherules and indicate where in the plume nucleation has occurred. Shortly after nucleation spherules are all approximately the same size. The growing crater and ejecta curtain are also shown. Figure 3.2.c (bottom) shows the expanding hemispherical vapor plume after 1000 seconds of expansion. The outer half of the vapor plume is labeled to indicate that quenching has occurred and the spherules are no longer growing. The spherules sizes are exaggerated to show that the outer portions of the vapor plume tend to have smaller spherules than the inner portions as described in section 3.3.6. The spherules in the portion of the plume labeled growing are shown as smaller than those in the quenched section to indicate that they have not yet reached their final size. The Earth and the dotted line are included to show how appropriate the approximation of a hemispherical vapor plume is at late times.
3.3.2 Expansion

In sections 3.3.2-3.3.5, we examine the adiabatic path followed by material in one representative cell. We focus on the vapor plume created by a 10km diameter impactor, impacting with velocities \( V_{\text{imp}} \) of 21 km/s and 30 km/s. As previously mentioned the vapor plume is partitioned into 160 equally massive hemispherical cells. Within these vapor plumes, we focus on the material in cell 80 out of 160. We choose cell 80 because it corresponds roughly to the average properties of the vapor plume at any given time. We choose a 10km diameter impactor because it roughly corresponds to the Chicxulub impactor. We chose 21 km/s because the resultant spherules agree with observation well, and because the velocity is similar to the average impact velocity of asteroids on Earth. We chose to make an in-depth comparison of 21 km/s and 30km/s impact velocities to illustrate those aspects of spherule formation that can be generalized to any velocity, and those that cannot. The initial conditions of the two vapor plumes are outlined in Table 3.1.

Table 3.1 Initial Conditions of Vapor Plumes

Initial conditions of the vapor plumes produce by a 10km diameter impactor impacting with velocities of 21 km/s and 30 km/s.

<table>
<thead>
<tr>
<th>( V_{\text{imp}} )</th>
<th>Diameter</th>
<th>Internal Energy</th>
<th>Density</th>
<th>Temperature</th>
<th>Pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>21 km/s</td>
<td>10.8 km</td>
<td>55 MJ/kg</td>
<td>6550 kg/m(^3)</td>
<td>34,300 K</td>
<td>499 GPa</td>
</tr>
<tr>
<td>30 km/s</td>
<td>11.6 km</td>
<td>113 MJ/kg</td>
<td>7460 kg/m(^3)</td>
<td>67,000 K</td>
<td>934 GPa</td>
</tr>
</tbody>
</table>
At time $t = 0$, the hemisphere begins to expand into free space. The outer cells begin to expand first and a rarefaction wave starts to travel inward from the outer surface of the hemispherical vapor plume. The initially large pressure gradient between the vapor plume and free space leads to high initial accelerations of the outer cells. As the vapor plume expands the pressure gradient declines and the cells expand with a roughly constant velocity. The Lagrangian position of material is given exactly as

$$ r(t) = r(0) + < v > t, $$

where $< v >$ is the average velocity of the material from time zero to time $t$ and $t$ is the time since expansion began. The velocity of material in the vapor plume quickly accelerates to its maximal velocity in a time $t_{\text{accel}}$. If $t \gg t_{\text{accel}}$, then $< v > \sim v_M$, where $v_M$ is the material’s maximal velocity. Additionally, at late enough times, $v_M t \gg r(0)$, and

$$ r(t) \approx v_M t $$

The vapor plume’s fast acceleration to its maximal expansion velocity leads to a simple relationship between velocity and position at late times. We define a normalized position

$$ \eta \equiv r / R(t), $$

where $R(t)$ is the radius of the entire vapor plume. At late times the normalized position of a cell is constant and given by,

$$ \eta = \frac{v_M}{V_R} $$

Figure 3.3 indicates that, $V(\eta) = \eta V_R$, where $V_R = \dot{R}(t)$. This is the late time dependence expected for any vapor sphere expanding into free space (Zel’dovich and Raizer 1967). This linear relationship means that the outer portions of the vapor plume are moving the
fastest, and that the slowest portions of the plume are closest to the point of impact. After one second of expansion, the material in cell 80 reaches \( \sim 95\% \) of its maximal radial velocity of \( \sim 13.7 \) km/s for a 30km/s impact. Similarly cell 80 from a 21km/s impact reaches \( \sim 93\% \) of its maximal radial velocity of \( \sim 9.3 \) km/s after one second of expansion. The 30km/s impact has \( V_R = 27.3 \) km/s and the 21 km/s impact has \( V_R = 18.9 \) km/s. Cell 80 corresponds to \( \eta \approx 0.5 \) at late times for both impact velocities.

![Normalized Cell Velocity](image)

Figure 3.3 Normalized Cell Velocity

Normalized cell centered velocity is plotted against normalized radius for an impact velocity of 21 km/s and a 10 km diameter impactor. Each ‘+’ represents one of 160 cells. The position and velocity data is taken after 10,000 seconds of expansion.

3.3.3 Nucleation

Figure 3.4 displays the thermodynamic paths followed by the two vapor plumes after some initial expansion, once temperatures are below 6000K. In the partial pressure of
SiO₂ is plotted. This is because our code includes an equilibrium chemistry calculation and silica dissociates into SiO + O or SiO + \( \frac{1}{2} \) O₂ at high temperatures (Appendix A.4). In the figure, the adiabats progress from high temperature and early times on the right to low temperature and later times on the left. The figure includes the expanding vapor’s final approach to the coexistence curve as well as the processes of nucleation, growth, and quenching. A labeled arrow indicates the point where the coexistence curve is crossed and nucleation begins. In an equilibrium calculation, liquid begins to form the instant that material reaches the coexistence curve. After this, the adiabat never leaves the coexistence curve. In a real second-order phase transition, the vapor phase becomes metastable and can make a slight excursion past the coexistence curve. Homogeneous nucleation theory, described in appendix A.1, permits the exploration of this metastability.
Figure 3.4 Adiabatic Paths Showing Nucleation, Growth, and Quenching

The adiabatic paths that cell 80/160 follows for a 10km diameter impactor and impact velocities of 21km/s (top) and 30km/s (bottom) are plotted in temperature-pressure space. The dashed line is the liquid vapor coexistence curve, which has a dot at the end to represent the critical point. The solid line represents the ideal partial pressure of SiO\(_2\) in the cell. The ideal partial pressure is defined as the total pressure multiplied by the mole fraction of SiO\(_2\). The partial pressure is smaller than the total pressure at most times because silica dissociates into SiO + O or SiO + \(\frac{1}{2}\)O\(_2\) at high temperatures (Appendix A.4). Included are three labeled arrows indicating three of the four phases of spherule formation, which are outlined in Section 3.3.1. Total pressure is not plotted because it obscures the partial pressure curves.
For $V_{\text{imp}} = 21 \text{ km/s}$ in Figure 3.4, nucleation begins slightly before the ideal partial pressure of SiO$_2$ reaches the coexistence curve. In an ideal gas composed of multiple chemical species, the partial pressure is $P_{\text{SiO}_2} = P_{\text{tot}} x_{\text{SiO}_2}$ where $P_{\text{tot}}$ is the total pressure of the system and $x_{\text{SiO}_2}$ is the mole fraction of SiO$_2$. This definition of the partial pressure is only valid for ideal gases and only approximates the behavior of our system. As such, we only use the partial pressure for illustrative purposes and never for any calculations.

For this reason we feel that a more exact treatment of partial pressure only for the sake of nicer plots is unnecessary. Figure 3.5 illustrates that although nucleation seems to begin before this ideal partial pressure of silica reaches the phase curve, nucleation does not actually begin until the vapor density is larger than the vapor density on the coexistence curve. The density of SiO$_2$ can be shown to be $\rho_{\text{SiO}_2} = \rho_{\text{tot}} \gamma_{\text{SiO}_2}$ where $\gamma_{\text{SiO}_2}$ is the mass fraction of SiO$_2$. The density of SiO$_2$ is an exact calculation and as such the density is used in the calculation of the degree of supercooling and other aspects of the model.

Figure 3.5 also gives a more detailed view of the nucleation event and the excursion into a supersaturated system. In Figure 3.5, the curve for vapor density on the coexistence curve separates the region where material is all vapor and the region where the material is a 2-phase mixture. When the vapor crosses this curve, nucleation begins and small condensed clusters of silica molecules (nuclei) begin to form. If we do not include equilibrium chemistry, nucleation begins when the total density curve crosses into the two-phase region. The addition of equilibrium chemistry changes the temperature where nucleation begins by $\sim 300 \text{K}$. This temperature difference corresponds to a large
difference in surface energy and leads to larger spherules than in the case where equilibrium chemistry is not included.

![Graph showing density and temperature relationships](image1)

**Figure 3.5 Detail of Nucleation Event in Density-Temperature Space**

Small portions of the adiabats from Figure 3.4 are plotted in density-temperature space. The dashed line represents the vapor density on the coexistence curve. This line acts as a boundary between vapor and a two-phase system as indicated. The nucleation event is also marked with a labeled arrow. The curve for total density is also plotted to indicate the effect of adding equilibrium chemistry to our model.

The degree of supercooling ($\theta$) is given by,

$$\theta = \frac{T_{eq} - T}{T_{eq}}$$

where $T$ is the materials temperature and $T_{eq}$ is the temperature at which vapor in equilibrium with liquid will have the same density as the supercooled vapor. We
describe how $\theta$ is computed in appendix A.2. The degree of supercooling during the nucleation event (Figure 3.6), gives the most detailed view of the nucleation event. The degree of supercooling measures the deviations from the coexistence curve that are characteristic of real, metastable, phase transitions. The nucleation rate or rate that nuclei form depends exponentially on $\theta$. As nuclei form, vapor turns to liquid, releasing energy in the form of latent heat. Once the silica in the system crosses the coexistence curve, the degree of supercooling initially increases linearly with time. This linear increase occurs because initially the nucleation rate is very low. As such, latent heat is not released at a high enough rate to alter the thermodynamic path of the material. As the degree of supercooling increases both the growth rate and nucleation rate increase. Eventually when these rates are high, enough latent heat is released to increase the temperature of the two-phase material and forces the adiabat back to the coexistence curve. When the adiabat reaches the coexistence curve nucleation ceases. For the 21 km/s case, the nucleation event takes just over 1.5 ms and the degree of supercooling is near its maximum value for an even shorter time. The 30 km/s case takes just over 27 ms. Once nucleation is over, no more nuclei form, so that the number of nuclei in the cell remains constant.

At the end of the nucleation event the average spherule or nucleus is only ~12% of its final diameter or ~0.17% of its final mass for the 21km/s impact. For the 30 km/s impact, the average nucleus is ~14% of its final diameter or ~0.27% of its final mass. This means that spherules obtain most of their mass through the process of growth.
Figure 3.6 Degree of Supercooling During Nucleation

The degree of supercooling ($\theta$) during nucleation is plotted against time since nucleation has started. $t_{nuc}$ is the time at which nucleation starts. $t_{nuc} \approx 1.29$ s for the $V_{imp} = 21$ km/s case and $t_{nuc} \approx 4.21$ s for the $V_{imp} = 30$ km/s case. Each ‘+’ corresponds to the degree of supercooling during a single time step. This plot represents cell 80/160 of a vapor plume created by a 10km diameter impactor impacting at velocities of 21 km/s (left) and 30 km/s (right). In the left figure nucleation begins at $\theta \approx 0.0141$ instead of $\theta = 0$, when the coexistence curve is crossed. For numerical reasons nucleation begins at $\theta > 0$, once a threshold nucleation rate has been reached. Our results are extremely insensitive to this necessary threshold as discussed in appendix A.2.

3.3.4 Growth and Quenching

After nucleation has ceased, the vapor continues to condense onto the existing nuclei, releasing latent heat. This condensation causes the nuclei to grow to macroscopic sizes. The growth process forces the adiabat to move along the coexistence curve in a robust way. If the adiabat goes above the coexistence curve in pressure-temperature space, the degree of supercooling increases, which causes the growth rate to increase. This increases the rate of latent heat release, forcing the adiabat back to the coexistence curve. Similarly,
if the adiabat goes below the coexistence curve, the degree of supercooling becomes negative and droplets shrink. This also forces the adiabat back to the coexistence curve. In Figure 3.4, for $V_{imp} = 21$ km/s, the adiabat follows the coexistence curve until ~1600K, after ~1000 seconds of expansion. At this point, quenching occurs, meaning that the adiabat leaves the coexistence curve because the growth rate has slowed to a point where latent heat release cannot force the adiabat to the coexistence curve. The growth rate is limited by the diffusion rate, or rate at which vapor molecules collide with spherules. When quenching occurs, the vapor has become so sparse that collisions between the growing spherules and vapor become rare.

When the adiabat leaves the coexistence curve at ~1600K, the average spherule is ~98% of its final diameter or 95% of its final mass. For $V_{imp} = 30$ km/s, quenching occurs around 1700K after ~430 seconds of expansion. At this point the average spherule is ~97% of its final diameter and 91% of its final mass. Once the adiabat leaves the coexistence curve, growth is essentially halted. The process of quenching leaves a certain amount of vapor in the system that will never condense. Even after 10,000 seconds of expansion, ~44% of the vapor is left uncondensed for the 21km/s impact and ~60% of the vapor is left uncondensed for $V_{imp} = 30$ km/s case. We will discuss the fate of the uncondensed vapor in the discussion section.

The size distribution in cell 80 is plotted in Figure 3.7. For $V_{imp} = 21$ km/s, the distribution is strongly peaked around the average value of 232 μm and has a standard
deviation of 7.3 \( \mu m \). For the 30 km/s case, the distribution is peaked around the average value of 725 \( \mu m \) with a standard deviation of 28 \( \mu m \). The time of nucleation in Figure 3.7 progresses right to left. This relation is expected, because the spherules created at earlier times had more time to grow when the degree of supercooling was high and as such are larger than those created at later times. Considering this time dependence, we find there is an obvious similarity between Figure 3.6 and Figure 3.7. This similarity indicates that changes in the nucleation rate are dominated by changes in the degree of supercooling.

Figure 3.7 Spherule Size Distribution in Cell 80

The distribution of spherules in cell 80 is plotted as a histogram of the number of spherules at a given diameter. Each ‘+’ corresponds to one of fifty equally spaced bins. The droplet sizes are plotted after 10,000 seconds of expansion, well after growth has ceased, not at the time of nucleation. This plot represents cell 80/160 of a vapor plume created by a 10km diameter impactor impacting at velocities of 21 km/s (left) and 30 km/s (right).
3.3.5 Spatial/Temporal Dependence

Although it is illustrative to look at one cell in detail, it is also important to understand what happens in the vapor plume as a whole. The initial condition of a homogeneous hemisphere ensures that all of the material follows the same adiabatic path during the expansion phase. This means all of the material in the vapor plume will cross the coexistence curve at the same point, and have identical surface energies, vapor densities, etc. The only difference is the rate at which material follows the release adiabat. In Figure 3.8 the time when nucleation begins in a cell is plotted against the cell’s normalized position. Nucleation generally begins in the outer, faster moving, cells before the inner, slower moving, cells. The innermost cells from the \( V_{imp} = 21 \text{ km/s} \) case are an exception to this rule. Intuitively we might expect that cells with the largest radial velocities will expand the fastest, but this is not always the case. The details of the volume expansion rate cannot be solved analytically (Zel’dovich and Raizer 1967).
Figure 3.8 Time of Nucleation versus Location in the Plume

For each cell the time at which nucleation starts, $t_{\text{nuc}}$, is plotted against its normalized position. Each ‘+’ corresponds to one of 160 cells. This plot represents the vapor plume created by a 10km diameter impactor impacting with velocities of 21 km/s (left) and 30 km/s (right).

Figure 3.9 shows how the average spherule size depends on where they form in the plume. The fast outer cells tend to create the smallest spherules and slow inner cells the largest. Figure 3.10 shows that although the spherule size depends on where the spherules are created in the plume, the size distribution is strongly peaked around the average value. For $V_{\text{imp}} = 21$ km/s the average spherule diameter for the entire plume is 217 $\mu$m with a standard deviation of 47 $\mu$m. For $V_{\text{imp}} = 30$ km/s the average spherule diameter for the entire plume is 689 $\mu$m with a standard deviation of 156 $\mu$m. Currently, in the K-Pg boundary layer, there are no measurements of variability of average spherule size with the distance they are found from the Chicxulub impact structure. Our model predicts a variation of more than 100 $\mu$m, which should be measurable and would act as a
verification of the model. Although this variation has not been measured, it is possible
that it has been previously overlooked.

Figure 3.9 Spherule Diameter versus Location in the Plume

The average spherule diameter, by mass, in each cell is plotted against the normalized
radius of each cell. Each ‘+’ corresponds to one of 160 cells equally massive cells. This
data is taken after 10,000 seconds of expansion, well after growth has ceased. This plot
represents the vapor plume created by a 10km diameter impactor impacting with
velocities of 21 km/s (left) and 30 km/s (right).

When comparing Figure 3.9 to Figure 3.8 a linear relationship between nucleation time
($t_{nuc}$) and spherule size is apparent for the 30 km/s impact velocity but not for the 21
km/s impact velocity. The adiabatic relation shown below can be used to understand the
dependence of spherules size on nucleation time,

$$ T \rho^{1-\gamma} = \text{const}, $$

or

$$ T \propto \rho^{y-1} $$

where $T$ is the temperature of the material, $\rho$ is the density, and $\gamma$ is the ratio of specific
heats. The nucleation time can be solved directly when we consider that for a given
impact velocity, all the material in the vapor plume crosses the coexistence curve at the 
same density,

$$\rho_{\text{cross}} = \rho = \frac{3M}{4\pi(R_{\text{out}}^3 - R_{\text{in}}^3)}$$

where $R_{\text{in}}$ and $R_{\text{out}}$ are the outer and inner radius of a cell at time $t_{\text{nuc}}$ and $M$ is the mass 
of the cell. As shown in section 3.3.2 late enough times, $t \gg t_{\text{accel}}$, material is located at 
a position $R(t) = v_m t$, where $v_m$ is the materials maximum radial velocity. Now if 
$t_{\text{nuc}} \gg t_{\text{accel}}$ then $R_{\text{in}} \approx V_{\text{in}} t_{\text{nuc}}$ and $R_{\text{out}} \approx V_{\text{out}} t_{\text{nuc}}$ and 

$$\rho_{\text{cross}} \propto t_{\text{nuc}}^{-3}$$

For cell 80, $t_{\text{accel}} \sim 1$ s for both 21 km/s and 30 km/s while $t_{\text{nuc}} = 1.29$ s for 21 km/s 
impact velocity and $t_{\text{nuc}} = 4.21$ s. We conclude that at the time when nucleation occurs, 
the $t_{\text{nuc}} \gg t_{\text{accel}}$ approximation is valid for the 30 km/s impact velocity but not for the 
21 km/s impact. Using the adiabatic relationship and the time dependence of $\rho_{\text{cross}}$ we 
find that

$$T \propto t_{\text{nuc}}^{3-3\gamma}$$

and

$$\frac{dT}{dt} \propto t_{\text{nuc}}^{2-3\gamma}$$

For small deviations from the phase curve when the $t_{\text{nuc}} \gg t_{\text{accel}}$, 

$$\dot{\theta} \propto \left(\frac{dT}{dt}\right)/T \propto t_{\text{nuc}}^{-1}$$

and is independent of $\gamma$. 
In Figure 3.6, the degree of supercooling increases linearly with time until $\theta$ is close to a maximum. This means $\dot{\theta}$ is a constant for a given cell. Because the material is losing internal energy at a rate $\frac{dU}{dt} \propto \frac{dT}{dt} \propto \dot{\theta}^{3y-2}$, we expect cells with a larger $\dot{\theta}$ will require more latent heat to be released in order to force the adiabat back to the coexistence curve.

Figure 3.11 shows that,

$$\frac{1}{\dot{\theta}} \propto d_{sp}$$

and when $t_{nuc} \gg t_{accel}$

$$\frac{1}{\dot{\theta}} \propto d_{sp} \propto t_{nuc}$$

where $d_{sp}$ is the average diameter of spherules in a given cell. We also know that the initial size of nuclei is inversely proportional to the degree of supercooling, while nucleation rate depends exponentially on the degree of supercooling. As such, small changes in the maximum degree of supercooling will have little effect on the size of nuclei produced, but a large effect on the nucleation rate. So all of the nuclei created in the plume are roughly the same size when nucleation ceases. This means the amount of latent heat required to force an adiabat back to the coexistence curve is given by,

$$\Delta U_l \propto M_{liq} \propto N$$

where $M_{liq}$ is the mass that condenses to liquid during the nucleation event and $N$ is the number of spherules. We find that every cell ends up with roughly the same mass fraction of the condensed phase and because all of the cells are equally massive, the number of nuclei created in a cell is

$$N \propto \frac{1}{d_{sp}^3} \propto \dot{\theta}^3$$
and when $t_{nuc} \gg t_{accel}$,

$$N \propto t_{nuc}^{-3}$$

As figure 3.12 shows $N$ actually scales as $\dot{\theta}^\alpha$ where $\alpha < 3$. We see a difference because the nuclei grow quickly during the nucleation event, when the degree of supercooling is high. This makes our assumption that all spherules are the same size when nucleation ends incorrect. Although only approximate, the relationship between the number of nuclei created leads to an interesting conclusion about the amount of latent heat required to force an adiabat back to the coexistence curve.

$$\Delta U_l \propto \dot{\theta}^3$$

and when $t_{nuc} \gg t_{accel}$,

$$\Delta U_l \propto \dot{\theta}^3 \propto t_{nuc}^{-3}$$

For all of out model runs we find when $t_{nuc} \gg t_{accel}$, as an analytical approximation, $d_{sph} \propto t_{nuc}$ and approximately, $N \propto t_{nuc}^{-3}$. More generally though, at any $t_{nuc}$, $d_{sph} \propto \frac{1}{\dot{\theta}}$ and approximately, $N \propto \dot{\theta}^3$. It is important to emphasize that these relations are only valid for material shocked to the same point on the Hugoniot curve. As such the relations can only be used to compare different cells within a given initially homogeneous vapor plume or to relate the vapor plume created by different size bodies impacting with the same velocity. With this caveat in mind, these important results directly link spherule size to the expansion rate of the vapor plume. Since this result applies to the entire vapor plume, not just the average properties, it provides an intuitive description of the nucleation process within the vapor plume. The expression tells us that smaller nuclei are formed earlier in the outer quickly expanding portions of the vapor
plume. It also directly links spherules size directly to the size of the impactor as described in the next section. The dependence on $t_{nuc}$ that we report is identical to the dependence reported by Ražer (1960) for the average properties of the vapor plume. Although the many approximations used by Ražer (1960) may have lead to inaccurate results, the fact that this dependence was determined over 50 years ago is impressive.

Figure 3.10 Spherule Size Distribution in Plume

The mass of spherules of a given diameter, in the entire vapor plume, is plotted as a histogram. Each ‘+’ correspond to one of fifty equally spaced bins. This plot represents the vapor plume created by a 10km diameter impactor impacting with velocities of 21 km/s (left) and 30 km/s (right).
Figure 3.11 Average Spherule Diameter versus the Inverse of the Rate of Change of the Degree of Supercooling

The average spherule diameter in each cell is plotted against the inverse of the rate at which the degree of supercooling is changing illustrating their linear relationship. Each ‘+’ corresponds to one of 160 cells. This plot represents the vapor plume created by a 10km diameter asteroid impacting with velocities of 21 km/s (left) and 30 km/s (right).

Figure 3.12 Number of Spherules Depends as a Function of the Rate of Change of the Degree of Supercooling

The logarithm of the total number of spherules in a cell is plotted against the logarithm of $\dot{\theta}$ when nucleation begins for each cell. Each dot corresponds to one of 160 cells for an impact velocity of 30 km/s, while each ‘+’ corresponds to one of 160 cells for an impact velocity of 21 km/s. Both data sets are for the vapor plume created by a 10km diameter impactor. This plot illustrates the dependence, $N \propto \dot{\theta}^\alpha$ where $\alpha$ is the indicated slope obtained with a linear fit of each data set.
3.3.6 Impactor Size and Velocity Dependence

In the previous section we saw that a higher $\dot{\theta}$ corresponds to smaller spherules. In this section we explore the relationship between spherule size and impact velocity, which is more complex. When impact velocity is increased we end up with larger $\dot{\theta}$. This increase in $\dot{\theta}$ comes from the increased volume expansion rate, which is a result of the increased initial internal energy and radial expansion velocity. As we saw previously, the increased $\dot{\theta}$ tends to make spherule sizes smaller. Figure 4 and 5 illustrate another important effect; as the impact velocity increases, the temperature at which an adiabat crosses the coexistence curve decreases. This decreased temperature leads to an increase in the surface energy that tends to make larger spherules (Appendix A.3). It is not easy to determine which of these competing effects will dominate and as such, the average spherule size has a complex dependence on impact velocity.

In Figure 3.13, the average spherule size for the entire vapor plume is plotted against impact velocity for impactor sizes that range from the smallest impacts on Earth to those which are planetary scale. The figure illustrates how these two counteracting effects, of increased surface energy and increased expansion rate, determine the spherule size. From an impact velocity of 15 km/s to ~28 km/s the effect of increasing the surface energy dominates. So as impact velocity increases, the average spherule size does as well. At impact velocities greater than ~28 km/s the effect of the increasing expansion rate dominates and the trend is reversed.
Figure 3.13 also illustrates the effect of changing the impactor size. In general, the average spherule diameter depends almost linearly on impactor diameter. We can understand this simple dependence by considering hydrodynamic similarity. If we neglect gravity, the equations of hydrodynamics are invariant under the following scale transformation,

\[ t' = \beta t, \quad x' = \beta x, \quad \text{and} \quad \rho' = \rho \]

where \( t \) is time, \( x \) is the position coordinate, \( \rho \) is density, and \( \beta \) is a scaling parameter. From this scaling we can conclude that if material in a vapor plume of initial size \( R_0 \) at initial position \( x_0 \) would come to the coexistence curve at time \( t_{nuc} \), then material at position \( \beta x_0 \) in a vapor plume size \( \beta R_0 \) will come to the coexistence curve at time \( \beta t_{nuc} \). The scaling of \( t \) and \( x \) indicates that material will have the same radial velocity, but \( \theta \propto 1/t_{nuc} \propto \frac{1}{d_{zph}} \), will be smaller by a factor of \( 1/\beta \) for the larger vapor plume so the spherules will be larger by a factor \( \beta \).
Figure 3.13 Average Spherule Size Created by Different Impact Conditions

The average spherule diameter for the entire vapor plume is plotted against the impact velocity. ‘+’s mark actual data points. The diameters of the impactors that the various curves correspond to are labeled in the legend. All data is taken at a time $t_{\text{stop}}$, which is roughly 10 times the time at which growth stops. This time is given by $t_{\text{stop}} \sim D_{\text{imp}} \times 1000 \text{ s}$, where $D_{\text{imp}}$ is the impactor diameter in km.

Due to quenching, only a fraction of the material in the vapor plume condenses into spherules. Figure 14 shows the amount of material that condenses and demonstrates how the amount changes with impact velocity. In general a smaller fraction of material condenses at higher impact velocities. The increased expansion velocity associated with a larger impact velocity makes quenching happen earlier. The earlier quenching corresponds to less overall growth and therefore less material condensed. Although the
curve for % impactor is more complex, it exhibits a general increase with increasing impact velocity. It is important to note that the % impactor curve corresponds to the mass condensed normalized by the mass of the impactor and does not correspond to the % of extraterrestrial material condensed. These two curves allow the reader to determine the mass in the vapor plume as well as the mass condensed at different impact velocities.

Figure 3.14 Condensed Mass as a Function of Impact Velocity

The solid curve corresponds to the mass condensed divided by the total mass of the vapor plume and is plotted as a percentage at varying impact velocities. ‘+’s mark actual data points. Similarly the dashed curve is the mass condensed divided by the mass of the impactor. For this particular plot the impactor is a 10km in diameter sphere with a density of 2500 kg/m³. All data points are taken after 10,000 seconds of expansion well after quenching has occurred and growth has stopped.
3.4 Discussion

Based on the estimated amount of iridium in the K/Pg boundary layer, the impactor that produced the Chicxulub crater is estimated to be a ~10km-15km diameter asteroid (Alvarez et al. 1980). The global layer is composed of ~250 μm diameter spherules in a clay matrix (Smit 1999). We find that a 10km diameter impactor creates spherules with an average size of 217 μm with a standard deviation of 47 μm for an impact velocity of 21 km/s. A 15km diameter impactor makes similar size spherules at ~20.5 km/s impact velocity. This velocity estimate is consistent with typical impact velocities of asteroids. We feel that this agreement with the estimated impactor size and impact velocity range demonstrates the efficacy of our model. We admit that this is not a statistically robust test but, impacts where impactor size is well constrained are rare.

It is important to comment on the limitations of our current model and the expected changes a more detailed model might produce. Although the assumption of a homogeneous spherical vapor plume that is initially at rest are approximately correct, 2D and 3D hydrocodes indicate that the vapor plume has a more complex geometry and lower expansion rates than our idealized model. (Pierazzo, Kring, and Melosh 1998) The only way to accurately model the more complex geometry of the vapor plume created by an impact would be to use a 2D or 3D hydrocode. By adapting this model to a higher dimensional code, we would be able to model the impact and the vapor plume it produces while leaving the number of assumptions at a minimum. Coupling the current model with a more realistic hydrocode simulation will probably be computationally intensive. As
discussed in section 3.6, a lower volume expansion rate corresponds to larger spherules. Qualitatively we expect the inclusion of a realistic geometry, gravity, and an atmosphere would tend to decrease the volume expansion rate, which should increase the size of the spherules. We also expect that these inclusions would cause quenching to happen later and more vapor would condense onto the existing spherules making them larger. This means the estimate of a 21 km/s impact velocity is probably an upper bound, assuming our expression for surface energy is accurate.

It is also important to discuss the differences we would expect if we used a more realistic target and impactor composition. As we discussed in the introduction, we expect the Chicxulub impactor was probably mafic. For gabbro which represents this mafic composition well, the Hugoniot curve has only been explored up to pressure of ~100 GPa (Trunin et al. 2001). For silica, vaporization and spherule formation do not occur until shock pressure of ~300 GPa. Although the Hugoniot of more realistic mafic material is not well know in the region of interest, we expect that it should be somewhat similar to that of pure silica. Assuming the two Hugoniot curves are identical, differences in the liquid vapor coexistence curve and the surface energy can change our results significantly. The surface energy of silica at 1500K is 298 N/m while the surface energy of basalt sample OFZ-P5 is 366 N/m at the same temperature (Boča et al. 2003, Walker and Mulins 1981). We do not expect basalt and silica to have the same coexistence curve and critical point or the same temperature dependence of surface energy. It is possible that the critical point of basalt is at a somewhat higher/lower temperature and pressure
than that of silica. This difference could lead to lower/higher impact velocities required to vaporize material.

However, if we do assume the critical points and release adiabats of the two materials are identical, we find the difference in surface energy will make basaltic spherules larger by a factor that is less than two. Due to the strong dependence of spherule size on impact velocity, basaltic spherules that are ~250 μm in diameter and consistent with those found in the K/Pg boundary layer will be created at an impact velocity of ~20 km/s instead of the 21 km/s reported for pure silica spherules. In order to extend this model to more realistic materials, a robust equation of state that can be tested against experiment is needed. It is also clear that this model would benefit greatly from an experimentally constrained expression for the temperature dependence of the surface energy of silica and other rocky materials at high temperatures.

Because we approximate the vapor plume as being composed only of material from the isobaric core, we cannot use Figure 14 to estimate the size of the impactor based on the total mass of resultant spherules. The inclusion of material outside of the isobaric core should increase the overall mass of the vapor plume. The addition of material of differing shock levels should also lead to spherules with a larger range in sizes. Keeping this limitation in mind it is still interesting to compare the results from Figure 14 to observables. For a Chicxulub like impact, with a 10 km diameter impactor and an impact velocity of 21 km/s, the isobaric core has a mass of $2.2 \times 10^{15}$ kg. The total condensed mass from this is $1.2 \times 10^{15}$ kg. If the impactor has a diameter of ~15 km then the isobaric
core has a mass of $7.3 \times 10^{15}$ kg which gives a condensed mass of $4.1 \times 10^{15}$ kg. Observationally the K/Pg boundary layer is about 3mm thick globally (Smit 1999). If we assume a bulk density of $\sim 2500$ kg/m$^3$ we find the layer has a total mass of $\sim 3.8 \times 10^{15}$ kg. Furthermore, approximately 50% of this layer is the clay matrix. So as a rough estimate the K/Pg boundary layer actually contains $\sim 1.9 \times 10^{15}$ kg of spherules. This estimate is close to the mass of spherules predicted to come from a slightly larger than 10km diameter impactor. It may also be important to consider that for a 21km/s impact velocity $\sim 25\%$ of the vapor plume’s mass is ejected at velocities greater than Earth’s escape velocity and so never falls back on the Earth.

Trying to compare our results to observation becomes more difficult when we consider what happens to the remaining uncondensed vapor when the vapor plume falls back onto Earth. Because the spherules do not have a significant differential velocity with respect to the gas we expect that even if some material escapes Earth, the fraction of condensed material to vapor will remain the same at $\sim 56\%$. This leads to an interesting discussion. When the remaining 44\% of vapor falls back onto earth it should eventually condense because SiO$_2$ is solid for the conditions at Earth’s surface. If the vapor condenses onto existing spherules, the predicted spherules would grow significantly. If we are still to end up with $\sim 250$ $\mu$m spherules, the original spherules would have to be smaller than 250 $\mu$m. This would make the predicted impact velocity of the Chicxulub impact slightly smaller than 20km/s.
It is also likely that when the vapor plume falls onto Earth’s atmosphere, the spherules decouple from the vapor plume thermodynamically and/or spatially. In this case, the vapor will condense by creating a second population of spherules. There are two basic ways this could happen and still agree with the observed K/Pg boundary layer. One way is that the secondary spherules are about the same size as the primary spherules. A more likely possibility is that these secondary spherules would be small, \( \leq 1 \mu m \), and be contained in or make up the clay matrix that surrounds the primary spherules. This might form a highly opaque “smoke” that would reflect much of the infrared radiation, produced by reentering spherules, onto the Earth’s surface, strongly increasing the surface heating (Goldin and Melosh, 2009). It should be possible to extend this model in the future to determine what happens to the remaining 44% of the vapor, as it falls back onto Earth’s atmosphere.
Appendix: Details of Nucleation and Chemistry

A.1 Homogeneous Nucleation and Growth

Classical Nucleation Theory described by Becker-Döring (1935) and Zel'dovich (1940) determines the metastability and kinetics of first order phase transitions. For our application, the theory describes how clusters (liquid droplets) grow over time through condensation and evaporation of single molecules. If we make the capillarity approximation, which states that the surface energy per unit area of a cluster is independent of its size, the free energy of formation for a cluster of size $r$ is given by

$$
\Delta F(r) = -\frac{4}{3} \pi r^3 n_{liq} \lambda m \theta + 4 \pi r^2 \sigma
$$

where $\lambda$ is the latent heat of fusion per unit mass, $m$ is the molecular mass, $\theta$ is the degree of supercooling defined as $\theta = \frac{T_{eq} - T}{T_{eq}}$, $n_{liq}$ is the number density of the liquid, $\sigma$ is the surface tension. The free energy $\Delta F(r)$ has a maximum, which can be solved for by setting the derivative $\frac{\partial \Delta F(r)}{\partial r} = 0$. The radius at which the maximum occurs defines the critical radius $r_{cr}$ given below.

$$
r_{cr} = \frac{2\sigma}{n_{liq} \lambda m \theta}
$$

Clusters smaller than this will evaporate and those larger than this will continue to grow. The steady state solution to the clustering equations attributed to Becker-Döring and Zel'dovich assumes that as critical clusters are created they are removed from the system and replaced by vapor. The steady state solution also assumes that the clusters and vapor
are in thermal equilibrium and that the droplets are large enough that thermal fluctuations associated with exchanging molecules are small. The solution, which we do not derive and simply state below, gives the number of clusters that are formed per molecule of vapor per unit time assuming that all thermodynamic variables are constant in time.

\[ I = D \kappa \exp \left( -\frac{\Delta F(r_{cr})}{k_b T} \right) \]

where \( k_b \) is Boltzmann’s constant, and \( D \) is the rate at which vapor molecules hit the spherical drop. Using kinetic theory, the flux rate of molecules onto any surface is \( \Phi = n_{vap} v_{th}/4 \), and \( D = \Phi \times Area \) (Blundell and Blundell 2006). So for a sphere

\[ D = \pi r_{cr}^2 n_{vap} v_{th} \]

where \( n_{vap} \) is the number density of the vapor and the thermal velocity of the vapor, \( v_{th} \), is given by:

\[ v_{th} = \left( \frac{8k_b T}{\pi m} \right)^{1/2} \]

The exponential factor is a Boltzmann factor, which describes the probability that thermal fluctuations will lead to the formation of critical clusters and \( \kappa \) is the Zel’dovich factor. \( \kappa \) is a direct result of solving the clustering equations. For a lucid explanation of the clustering equations and a derivation of the steady state solution, including the Zel'dovich factor, see Abraham (1974). If we write the free energy of formation as a function of \( N \), where \( N \) is the number of molecules in the cluster, through the relation

\[ N = \frac{4}{3} \pi r^3 n_{liq} \]

then
\[
\kappa = \sqrt{-\frac{1}{2\pi k_b T} \left(\frac{\partial^2 AF(N_{cr})}{\partial N^2}\right)} = \frac{1}{2\pi r_{cr}^2 n_{liq}} \sqrt{\frac{\sigma}{k_b T}}
\]

Which gives the expected

\[
l = \frac{n_{vap}}{n_{liq}} \left(\frac{2\sigma}{\pi m}\right)^\frac{1}{2} \exp\left(-\frac{4\pi r_{cr}^2 \sigma}{3k_b T}\right)
\]

In 1977 Katz and Weidersich showed that nucleation theory can be developed without assuming that droplets are in equilibrium with the vapor. The newer more accurate approach to homogeneous nucleation theory is described in detailed and solved by Girshick and Chiu (1990). This newer approach, coined kinetic nucleation theory, describes experimental data much better than classical nucleation theory. Kinetic nucleation theory gives a nucleation rate, \( I_{kin} \), which is different from the classical nucleation rate, \( I_{cl} \), as follows.

\[
I_{kin} = \frac{\exp(\xi)}{S} I_{cl}
\]

Where \( \xi \) is the dimensionless surface energy of a drop given by

\[
\xi = \frac{4\pi r_{cr}^2}{k_b T}
\]

and \( S \) is the supersaturation ratio which is shown by Mc Donald (1964) to be equivalent to

\[
S = \exp\left(\frac{\lambda m \theta}{k_b T}\right)
\]

Including this equivalence we find,

\[
I_{kin} = \frac{n_{vap}}{n_{liq}} \left(\frac{2\sigma}{\pi m}\right)^\frac{1}{2} \exp(\beta)
\]
where \( n_{vap} \) is the number density of the vapor, \( k_b \) is Boltzmann’s constant, and \( \beta \) is given below:

\[
\beta = -\frac{\lambda m \theta}{k_b T} + \xi - \frac{4\xi^3}{27} \left( \frac{k_b T}{\lambda m \theta} \right)^2
\]

To describe the size distribution created during a nucleation event we need to know the nucleation rate and critical cluster size as well as the rate at which supercritical clusters will continue to grow. Raïzer (1960) following Frenkel (1946) derived the growth rate of supercritical clusters as:

\[
\frac{dN}{dt} = D \left[ 1 - \exp \left( \frac{\Delta_{\Delta F}}{k_b T} \right) \right]
\]

Where

\[
\Delta_{\Delta F} = \Delta F(N + 1) - \Delta F(N)
\]

If we expand \( \Delta F(N) \) in Taylor series and neglect terms with higher than second order derivatives.

\[
\Delta_{\Delta F} = -\lambda m \theta + \frac{2}{3} \gamma N^{-\frac{1}{3}} - \frac{1}{9} \gamma N^{-\frac{4}{3}}
\]

Where

\[
\gamma = 4\pi \sigma \left( \frac{3}{4\pi n_{liq}} \right)^{\frac{2}{3}}
\]

We take the series out to second order derivatives because at \( r_{cr} \) or \( N_{cr} \), the first derivative of \( \Delta F(N) \) is zero. If the series only includes first order derivatives, clusters will never grow larger than the critical size. Our expression for \( \Delta_{\Delta F} \) differs greatly from the expression used by de Niem (2002) and Razier (1960) who ignored surface effects.
and approximated $\Delta_{AF} \approx -\lambda m \theta$. The expression they use is a good approximation when clusters are much larger than $r_{cr}$ but is quite inaccurate at the beginning of growth.

For simplicity in our code we use $\frac{dr}{dt}$ instead of $\frac{dN}{dt}$. To make this conversion we use the following equations.

$$N = \frac{4}{3} \pi r^3 n_{liq}$$

and

$$\frac{dN}{dt} = 4\pi r^2 n_{liq} \left( \frac{dr}{dt} \right)$$

Which lead to:

$$\frac{dr}{dt} = \frac{n_{vap} v_{th}}{n_{liq}} \frac{1}{4} \left[ 1 - \exp \left( -\frac{\Delta_{AF}}{k_b T} \right) \right]$$

### A.2 Numerical Solution of Nucleation Equations

A hydrocode is a finite difference method primarily used to model the effects of explosions and impacts. In this study we use a one dimensional Lagrangian hydrocode in which material remains in the same cell throughout the calculation. Since we do not have to consider relativistic velocities, Newton’s laws of motion sufficiently describe the motion of the material. Figure A.2 outlines a complete solution cycle of our 1D Lagrangian hydrocode. For a more in depth description of this method see Melosh (2007).
Figure A.1 Illustration of 1-D Lagrangian Hydrocode

Schematic illustration of a one-dimensional Lagrangian hydrocode computation. A single cell of this computation at an initial time \( t \) is shaded on the left half of the figure. The cell is bounded by two vertices, shown as heavy dots. Position \( x \), velocity \( v \), and mass \( m \), are defined at each vertex. Cell-centered quantities are pressure \( P \), internal energy \( E \), and density \( \rho \). The code advances from time \( t \) to \( t + \Delta t \) by using Newton’s laws of motion to compute acceleration of the vertices and hence the new velocity as well as \( x_i' \) and \( x_{i+1}' \) which gives us the new volume and density. The internal energy is then computed by determining the amount of work done on or by the cell. Then a new solution cycle begins again, each time using the equation of state to relate the new density and internal energy to temperature and pressure.

The other important aspect of our model is the addition of nucleation and growth to the hydrocode. Once the system becomes supercooled, we choose a time step such that the change in thermodynamic variables from one step to the next is small. By doing this we can insure that thermodynamic variables within a given time step are essentially constant, and thus the steady state equation of nucleation is valid. Qualitatively a nucleation event should span many time steps. In the steady state limit, the number of clusters created in the \( n_{th} \) time step in one cell is.

\[
N_n = I \Delta t_n N_{vap}
\]
Where $N_{\text{vap}}$ is the total number of vapor molecules in the cell available to condense and $\Delta t_n$ is the size of the $n_{th}$ time step. The size of these new clusters range from,

$$r_{\text{min}}(n) = r_{cr} , \text{ to } r_{\text{max}}(n) = r_{cr} + \frac{dr}{dt} \Delta t_n$$

Because we allow $n_{\text{liq}}$ to be variable, the actual quantity we save is minimum and maximum mass of the clusters.

The size of clusters created in previous time steps in this cell are also updated such that for all $i < n$.

$$r_{\text{min}}(i) \rightarrow r_{\text{min}}(i) + \frac{dr}{dt} \Delta t_n$$

$$r_{\text{max}}(i) \rightarrow r_{\text{max}}(i) + \frac{dr}{dt} \Delta t_n$$

Although the model assumes that the clusters made during a given time step are distributed equally between $r_{\text{min}}$ and $r_{\text{max}}$, the total size distribution in the cell has contributions from each time step where nucleation has occurred, as shown in Figure 7.

The average mass of a single cluster created in time step $i$ is

$$< m_i > = \frac{\pi}{3n_{\text{liq}}} \left( \frac{r_{\text{max}}^4(i) - r_{\text{min}}^4(i)}{r_{\text{max}}(i) - r_{\text{min}}(i)} \right)$$

Then the mass of liquid in a cell is

$$M_{\text{tot}} = \sum_{i=1}^{n} < m_i > N_i$$
The ANEOS equation of state for SiO$_2$ developed by Melosh (2007) is used to solve for all thermodynamic variables at every time step except for surface energy $\sigma$ which has to come from experimental data. As a default, ANEOS equation of state assumes that a system is in equilibrium and thus any 2-phase system will lie on the coexistence curve.

To remedy this default of ANEOS we simply input the liquid mass fraction calculated above into ANEOS and allow the calculation to stray from the coexistence curve. This simple change allows ANEOS to relate temperature and density to energy and pressure for metastable systems.

To calculate the nucleation rate, we must also calculate the degree of supercooling. The degree of supercooling ($\theta$) as previously described is given by,

$$\theta = \frac{T_{eq} - T}{T_{eq}}$$

where $T$ is the materials temperature and $T_{eq}$ is the temperature at which vapor in equilibrium with liquid will have the same density as the supercooled vapor. As we stated earlier the equation of state relates density and temperature to pressure and internal energy. As a default, ANEOS assumes that material is in equilibrium on the coexistence curve. So in order to get $T_{eq}$, we use the default ANEOS calculation and vary temperature and total density, until the vapor density is equal to the supercooled vapor density. This temperature is then $T_{eq}$.

For numerical reason we must set a threshold nucleation rate which must be surpassed in order for nucleation to occur. Luckily, during a nucleation event the nucleation rate
spans several orders of magnitude and a vast majority of the clusters are created when $\theta$ is a maximum, this makes our results extremely insensitive to what we choose for our threshold rate, as long as $I_{\text{threshold}}$ corresponds to a $\theta_{\text{threshold}} < \theta_{\text{max}}$.

A.3 Surface Energy

The ANEOS equation of state for SiO$_2$ developed by Melosh (2007) is used to solve for all thermodynamic variables at every time step except for surface energy $\sigma$ which has to come from experimental data. The nucleation rate has a strong exponential dependence on surface energy and therefore sensitive to the expression used to describe the surface energy. In the temperature range that has been explored experimentally, 723K to 2073K, the surface energy of SiO$_2$ is roughly constant, $\sigma \sim 0.3$ N/m (Parikh 1958, Boča et al. 2003). For this reason previous works have not taken the temperature dependence of surface energy into account. For most materials, surface energy decreases with increasing temperature. In the case of liquid silica the dissociation of $2\text{SiO}_2 \rightarrow \text{Si} + \text{SiO}_4$ causes the surface tension to slightly increase with increasing temperature even at temperatures of up to 2073K (Boča et al. 2003). However, as the temperature approaches the critical temperature, the surface energy vanishes for any material. The critical temperature for silica is $T_c \approx 5379K$ as described by ANEOS. Many materials are known to have a temperature dependent surface energy given by $\sigma = \sigma_0 (T - T_c)^{\frac{11}{9}}$ where $\sigma_0$ is a constant (Guggenheim 1945). For this reason and the sake of simplicity, we model the surface energy as shown below.
\[ \sigma(T) = \begin{cases} 
0.3 \frac{N}{m} & \text{if } T \leq T_t \\
\sigma_0 (T_c - T)^{11/9} & \text{if } T > T_t 
\end{cases} \]

Where \( T_t \) is some transition temperature and \( \sigma_0 \) is set so that the function is continuous at \( T_t \). Molecular dynamics studies of SiO\(_2\) cluster indicates that \( T_t \) lies somewhere between 3000K and 3500K (Schwei
gert et al. 2002). In Figure A.2 we plot two expressions for surface tension using \( T_t = 3000K \) and \( T_t = 3500K \).

![Figure A.2 Surface Energy versus Temperature](image)

The temperature dependent expression for surface energy is plotted for the transitional temperatures, \( T_t = 3000 \text{ K} \) and \( T_t = 3500 \text{ K} \).

We have performed calculations for a 10km diameter impactor using both of these values for \( T_t \) in order to understand the effect of changing the surface energy model (Figure A.3). As we expect the \( T_t = 3500K \) model creates larger spherules until an impact velocity greater than \( \sim 33 \text{ km/s} \). At these high impact velocities, material crosses
the liquid vapor coexistence curve at temperatures lower than 3000K so that both models give the same surface energy. For the rest of the calculations we only used $T_t = 3000$K. We admit an obvious lack of experimental data and hope that our work will spur further research regarding the surface energy of SiO$_2$ at high temperatures.

![Figure A.3 Spherule Diameter versus Impact Velocity for Transition Temperatures](image)

Figure A.3 Spherule Diameter versus Impact Velocity for Transition Temperatures

The average spherule diameter is plotted against impact velocity for two different expressions for the temperature dependence of the surface energy of silica. The ‘+’s mark model output. This data corresponds to a 10km diameter impactor. All data points are taken after 10,000 seconds of expansion well after quenching has occurred and growth has stopped.

### A.4 Vapor Phase Chemistry

At high temperature SiO$_2$ vapor tends to dissociate, SiO$_2$ → SiO + $\frac{1}{2}$O$_2$ → SiO + O → Si + 2O. ANEOS allows for molecules and dissociation but it does so by introducing an effective binding energy so we have no knowledge of the abundance of these various
species. Initial equilibrium chemistry calculations using HSC Chemistry program 5.0 (Roine 2002) indicate that when nucleation occurs the system consists of a mixture of these species. In order to accurately determine the degree of supercooling, $\theta$, we have to know exactly how much SiO$_2$ is in the system. We do this by including an equilibrium chemistry calculation in the hydrocode that uses the BNR algorithm. The BNR (Brinkley, NASA, RAND) algorithm is a second-order method, which finds the abundance of different chemical species that will minimize the Gibbs free energy at a given pressure, temperature, and elemental abundance. For a description of the BNR algorithm, see Smith and Missen (1982). All of the thermochemical data used in the calculation is obtained from the NIST-JANAF Thermochemical Tables (Chase 1998). Figure 5 illustrates the importance of including equilibrium chemistry calculations.

It has been suggested that it may be important to also consider the reaction SiO + $\frac{1}{2}$O$_2$ $\rightarrow$ SiO$_2$ on the surface of critical cluster (Katz and Donohue 1982). This process becomes important when the reaction rate becomes comparable to the diffusion rate of SiO$_2$ onto the surface of a cluster. This surface reaction rate depends on both the rate of adsorption of SiO and O$_2$ onto the cluster and the rate at which adsorbed SiO and O$_2$ come into contact. These rates need to be determined experimentally before they can be included in a calculation with any accuracy. Although these rates have not yet been experimentally determined, we argue that surface reactions do not need to be included in our model. When nucleation occurs in our models about one third of the silicon atoms are in the form of SiO$_2$ and the other two thirds is in SiO. We conclude that at such high partial pressure
\[ P_{SiO_2} \sim 0.01 - 0.1 \text{ GPa} \]

the diffusion rate of SiO\(_2\) to the cluster will be much higher than the surface reaction rate. As such we assume that any contributions to nucleation rates due to surface reactions on a clusters are minimal. Original calculations by Katz and Donahue (1982) show that even if the surface reaction rate is very high and the partial pressure of SiO\(_2\) is a very small fraction of the SiO partial pressure, the temperature where nucleation begins is only changed by \( \sim 35\text{K} \). This difference in nucleation temperature most likely has a smaller effect on our results than the uncertainty in the SiO\(_2\) coexistence curve and our expression for surface energy. If we were to include this effect we would expect a smaller degree of supercooling would be required to have a significant nucleation rate. This change would then tend to make slightly larger nuclei because 

\[ \tau_{cr} \propto 1/\theta . \]

### A.5 Kinetically Frustrated Nucleation

We expect in an adiabatic expansion that the coexistence curve can only be followed for so long and eventually quenching will occur. Initially when quenching occurred, the nucleation equations would predict a secondary nucleation event. This secondary event indicates that at a high degree of supercooling, vapor condenses into new nuclei rather than onto existing spherules. de Neim (2002) reports a similar spurious result, with several nucleation events. Under further scrutiny, we find this result is an unphysical oversight.

Ražer (1960) determined that the time it takes a critical cluster to form is given by \( \tau_n = N^2/4D \) where \( N \) is the number of molecules in a critical cluster and \( D \) is the rate
at which vapor molecules collide with a critical nucleus. The formation time is a result of the random nature of the condensation and evaporation that occurs during the creation of a critical cluster. In order to use the steady state approximation, this time should be much smaller than the time scale at which thermodynamic variables change. We use $\tau_\rho$ which is defined such that the $\rho (t_o + \tau_\rho) = \rho(t_o)/2$, where $\rho (t)$ is the density of the vapor, to describe the timescale at which thermodynamic variables change. In order to create any critical nuclei, a Boltzmann distribution of clusters needs to be established before the system changes significantly, or $\tau_\rho/\tau_n \gg 1$. If the system does not meet this criterion then thermal fluctuations do not have sufficient time to create clusters of critical size and we say that the system is kinetically frustrated. When the system is kinetically frustrated, supercritical clusters continue to grow but nucleation doesn’t take place. Even when we relax the criterion to be $\tau_\rho/\tau_n \geq 1$, we find our system is always kinetically frustrated when quenching occurs. As such when we include the criteria for kinetic frustration, multiple nucleation events do not occur in a cell.
Impact craters are the most obvious indication of asteroid impacts, but craters on Earth are quickly obscured or destroyed by surface weathering and tectonic processes (Simonson and Glass 2004). Thus, the Earth’s impact history is inferred either from estimates of the present-day impactor flux determined by observations of near Earth asteroids or from the Moon’s incomplete impact chronology (Ivanov and Hartmann 2007, Le Feuvre and Wieczorek 2011, Stuart and Binzel 2004). Fortunately, asteroids impacting the Earth typically vaporize a mass of target rock comparable to the projectile’s mass. As this vapor expands in a large plume or fireball, it cools and condenses into molten droplets called spherules (Johnson and Melosh 2012a). For asteroids larger than ~10 km in diameter, these spherules are deposited in a global layer. Spherule layers, if preserved in the geologic record, provide information about an impact even when the source crater cannot be found (Simonson and Glass 2004). Here we report estimates of the sizes and impact velocities of the asteroids that created global spherule layers. The impact chronology from these spherule layers reveals that the impactor flux
was significantly higher 3.5 Gyr ago than it is currently. This conclusion is consistent with a gradual decline of the post Late Heavy Bombardment impactor flux.

There have been several attempts to model the process of spherule formation in the hope that the properties of an impacting body could be determined from observations of the corresponding spherule layer. These simplified models indicated that spherule size depends strongly on the size of an impactor but suggested a weak dependence on the impact velocity (Raizer 1960, Melosh and Vickery 1991, O’Keefe and Ahrens 1982). A more detailed model contradicts these results and instead shows that the impact velocity, not the size of an impactor, is the main determinant of spherule size (Johnson and Melosh 2012a). Although we cannot use spherule size to deduce the size of an impactor, we can use the thickness of a spherule layer for the same purpose. We assume that, as with the K-Pg boundary, all spherule layers have a roughly constant thickness globally (Smit 1999). This means the total mass of spherules in the layer can be determined using only the thickness of the spherule layer and the fraction of spherule in the layer at one, or a few, representative locations.

We assume that, as with the K-Pg boundary, the thickness of all spherule layers is roughly constant everywhere on Earth (Smit 1999). The total mass of spherules in the layer can thus be determined using only the thickness of the spherule layer and the fraction of spherules in the layer.

$$M_{sp} = 4\pi R_e^2 \rho_{sp} \left(\frac{r_f}{2}\right)$$  \hspace{1cm} \text{(equation 4.1)}
where $M_{sp}$ is the mass of spherules in the layer, $R_e$ is the Earth’s radius, $\rho_{sp}$ is the spherule density, and $t_r$ is the reduced thickness of the spherule layer. We define the reduced layer thickness as the thickness that a spherule layer would have if it were composed of 50% spherules by volume, as most undisturbed layers are. In our definition of reduced layer thickness, the remaining volume in the layer is composed of pore space or matrix material. Thus, the reduced layer thickness can be determined using the following expression, $t_r = 2 f_{sp} t$ where $t$ is the measured layer thickness and $f_{sp}$ is the volume fraction of spherules in the layer.

To determine the size of an impacting body, we relate the total mass of the spherules in the layer to the mass of the impactor. For typical asteroid impact velocities on Earth, the mass of the vapor plume is dominated by material from the isobaric core (Johnson and Melosh 2012a). The isobaric core is the central, most highly shocked region of an impact. The material encompassed by the isobaric core is derived from a spherical region beneath the point of impact with a size comparable to the impactor and with a mass of about twice the impactor mass. This relationship holds for a wide range of impact velocities, target and impactor materials, and impact angles (Pierazzo et al. 1997). In a simple model where the vaporized material is initially at rest and expands above the target surface to fill a perfect hemisphere, ~25% of the material is ejected faster than Earth escape velocity for typical impact velocities of ~20 km/s (Johnson and Melosh 2012a). If quenching takes place, only a fraction (~50%) of the vapor actually condenses into spherules (Johnson and Melosh 2012a, Raïzer 1960). To include the uncertainty of how much vapor condenses
into spherules that fall back on the Earth we define a factor $\xi$ and define the total mass of spherules in the layer as:

$$M_{sp} = \xi M_{imp}$$  \hspace{0.5cm} (equation 4.2)

where $M_{imp}$ is the mass of the impactor and, $\xi$ is an efficiency factor that conservatively ranges from 0.5 to 2. When $\xi=2$ this means almost 100% of the vaporized material ends up as spherules in a global layer and $\xi = 0.5$ is a lower limit that accounts for quenching and material being ejected at velocities higher than Earth’s escape velocity. The mass of a spherical impactor is simply

$$M_{imp} = \frac{4}{3} \pi R_{imp}^3 \rho_{imp},$$

where $R_{imp}$ is the impactor’s radius and $\rho_{imp}$ is the density of the impactor. Using the mass of a spherical impactor, equations 4.1, equation 4.2, and assuming that $\rho_{sp} \approx \rho_{imp}$, we obtain equation 4.3.

$$D_{imp} = 17 \left( \frac{t_r}{\xi} \right)^{\frac{1}{3}}$$  \hspace{0.5cm} (equation 4.3)

where $D_{imp}$ is the impactor diameter in km and is an efficiency factor $\xi$ that conservatively ranges from 0.5 to 2 for typical asteroidal impact velocities on Earth. Additionally, $t_r$ is the layer’s reduced thickness in cm, defined as $t_r = 2 f_{sp}$ where $t$ is the measured layer thickness and $f_{sp}$ is the volume fraction of spherules in the layer.

We test the accuracy of equation 4.3 by comparing the impactor size estimated using spherule layer thickness with the impactor size determined by other methods. The K-Pg boundary layer is found at numerous sites globally and has a thickness of $\sim 3$ mm and is $\sim 50\%$ spherules by volume (Smit 1999). Using the entire range of $\xi$ we find $D_{imp} = 9.0 – 14$ km. This is consistent with 10 ± 4 km size of the Chicxulub impactor as determined by
Iridium fluence and similar estimates from the size of the Chicxulub impact structure (Alvarez et al. 1990, Collins et al. 2002). Our impactor size estimates for two other spherule layers S2 and S3 (table 4.1) are also consistent with the estimate of 3-7 times larger than the Chicxulub impactor also based on total Iridium fluence (Kyte et al. 2003). The estimates of impactor sizes using equation 4.3 are only valid if the data taken from a limited region are representative of the global spherule layer. Many spherule layers show signs of redeposition by surface processes and/or subsequent tectonic deformation, which both reduce the accuracy of the global thickness estimate (Lowe et al. 2003). In addition to this uncertainty, the assumption that these layers represent a global layer of vapor condensates may be incorrect. Some of these spherule beds may be composed of melt spherules created through the fragmentation of melt ejected during an impact. Melt spherules can be morphologically identical to vapor condensate spherules and may be ejected thousands of kilometers from the impact site (Smit 1999). One major difference between the two types of spherules is the dependence of the layer thickness and size of spheroidal particles as a function of distance from the point of impact. Both droplet abundance and particle size decrease strongly with distance from the impact for melt droplets, whereas for a vapor-condensate spherule layer these properties are more or less uniform globally (Smit 1999). This means that if a layer is found in several locations, it may be possible to distinguish between the two types of spherules. It may also be possible to determine whether a layer is composed of melt droplets if impact lapilli are present. These accretionary particles are found in association with melt droplets in the Chicxulub ejecta more than 2000 km from the source crater (Yancey and Guillemette 2008).
Table 4.1 The Earth’s Impact History From Spherule Layer Data

The columns in the table from left to right represent: the name of the spherule layer, the age of the layer, the reduced thickness of the layer, the average spherule size within the layer, the size of the impactor as determined by equation 4.3, and the impact velocity determined by the method described in Figure 4.1, measurements that indicate extraterrestrial origin (if they exist), and the reference from which various data were taken. In some cases multiple layers are attributed to the same impact. These layers have been indicated by *, o, or + after the name of the layer, where all layers with the same symbol are attributed to the same impact. In the column labeled ET. extraterrestrial origin is indicated by Ir and/or Cr where Ir means that the layer has a significant Iridium anomaly and Cr means that Chromium isotope data indicates an extraterrestrial origin. There are many other spherule layers that are known to be more proximal melt droplet layers that are not included in this table. When possible, we obtained spherule layer data from the 2004 review of known spherule layers by Simonson and Glass (2004) in an attempt to present a consistent interpretation of geologic data.

<table>
<thead>
<tr>
<th>Name</th>
<th>Age (Gyr)</th>
<th>( t_r ) (cm)</th>
<th>Average Spherule Size (mm)</th>
<th>Impactor Diameter (km)</th>
<th>Impact Velocity (km/s)</th>
<th>ET.</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>3.47</td>
<td>10-15</td>
<td>0.3 – 0.6</td>
<td>29-53</td>
<td>18.8-21.2</td>
<td></td>
<td>1, 2</td>
</tr>
<tr>
<td>S2</td>
<td>3.26</td>
<td>20</td>
<td>0.15 -2.5</td>
<td>37-58</td>
<td>17.7-25.6</td>
<td>Cr</td>
<td>1, 2</td>
</tr>
<tr>
<td>S3</td>
<td>3.24</td>
<td>30-35</td>
<td>0.6-1.5</td>
<td>41-70</td>
<td>20.6-22.8</td>
<td>Ir, Cr</td>
<td>2</td>
</tr>
<tr>
<td>S4</td>
<td>3.24</td>
<td>15</td>
<td>0.2-1.6</td>
<td>33-53</td>
<td>18.2-22.2</td>
<td>Ir, Cr</td>
<td>1, 2</td>
</tr>
<tr>
<td>Jeerinah*</td>
<td>2.63</td>
<td>0.1-0.5</td>
<td>0.5</td>
<td>6.3-17</td>
<td>21.9-25.1</td>
<td>Ir, Cr</td>
<td>13</td>
</tr>
<tr>
<td>Monteville*</td>
<td>2.60-2.65</td>
<td>10</td>
<td>0.65</td>
<td>29-46</td>
<td>20.4-21.4</td>
<td>Ir</td>
<td>1, 14</td>
</tr>
<tr>
<td>Reivilo*</td>
<td>2.56</td>
<td>2</td>
<td>~0.6</td>
<td>17-27</td>
<td>21.3-22.4</td>
<td>Ir</td>
<td>1, 15</td>
</tr>
<tr>
<td>Paraburdo*</td>
<td>2.57</td>
<td>2</td>
<td>~0.6</td>
<td>17-27</td>
<td>21.3-22.4</td>
<td>Ir</td>
<td>15, 16</td>
</tr>
<tr>
<td>Bee Gorge</td>
<td>2.54</td>
<td>0.1-1</td>
<td>0.56</td>
<td>6.3-21</td>
<td>21.7-26.1</td>
<td>Ir</td>
<td>17, 18</td>
</tr>
<tr>
<td>Dales Gorge*</td>
<td>2.49</td>
<td>12</td>
<td>0.6-0.8</td>
<td>31-49</td>
<td>20.1-21.7</td>
<td>Ir, Cr</td>
<td>1, 17, 19</td>
</tr>
<tr>
<td>Kuruman*</td>
<td>2.46-2.52</td>
<td>0.6</td>
<td>~0.6</td>
<td>11-18</td>
<td>22.3-23.8</td>
<td></td>
<td>20</td>
</tr>
<tr>
<td>Grænseso</td>
<td>1.85-2.13</td>
<td>40</td>
<td>0.5-1.0</td>
<td>46-73</td>
<td>19.1-21.3</td>
<td></td>
<td>1, 21</td>
</tr>
<tr>
<td>K-Pg</td>
<td>0.065</td>
<td>0.3</td>
<td>0.25</td>
<td>9.0-14</td>
<td>20.4-21.5</td>
<td>Ir, Cr</td>
<td>9, 22</td>
</tr>
<tr>
<td>Cpx</td>
<td>0.035</td>
<td>0.04</td>
<td>0.25-0.5</td>
<td>4.6-7.3</td>
<td>22.0-27.0</td>
<td>Ir, Cr</td>
<td>1, 23, 24</td>
</tr>
</tbody>
</table>

1 (Simonson and Glass 2004)  
2 (Lowe et al. 2003)  
3 (Rasmussen and Koeberl 2004)  
4 (Kohl et al. 2006)  
5 (Goderis et al. 2011)  
6 (Hassler et al. 2010)  
7 (Simonson et al. 2009a)  
8 (Simonson 1992)  
9 (Glikson and Allen 2004)  
10 (Simonson et al. 2009b)  
11 (Chadwick et al. 2004)  
12 (Shukolyukov 1998)  
13 (Glass et al. 1998)  
14 (Kyte et al. 2011)
Figure 4.1 Estimate of Impact Velocity for Layer S1

A graphical representation of how impact velocity is estimated for spherule layer S1. Spherule layer S1 is ~3.47 Gyr old and has a reduced thickness of 10-15 cm. Using Equation 3 and the reduced thickness we estimate that the spherule layer was created by a 29-53 km diameter impactor. The solid black curve represents average spherule size as a function of impact velocity for a 29 km diameter impactor. The dashed black curve represents average spherule size for a 53 km diameter impactor. Both of the black curves are obtained using the model for spherule formation in an expanding vapor plume of Johnson and Melosh (2012a). We have also plotted guides to the eye at 0.3 mm and 0.6 mm spherule diameter. This corresponds to the estimated range for the average spherule size in the layer. We then assume the impact has a typical asteroidal impact velocity of ~20 km/s and find the bounding velocities in this range are 18.8-21.2 km/s. In this case we neglect the other possible solution, a crossing that occurs at cometary impact velocities of 35-40 km/sec. We estimate the impact velocity for all of the other layers in Table 4.1 in a similar fashion. The model of Johnson and Melosh (2012a) is simple and strictly applies to spherules created from a pure silica impactor and target. Johnson and Melosh (2012a) suggest that impactor and target material may have a significant effect on the resultant spherule size.
Another way to discriminate spherule types is to determine whether a layer contains extraterrestrial material (Johnson and Melosh 2012a). Only vapor condensate spherules should contain significant extraterrestrial material, because the impactor is vaporized at typical Earth impact velocities. Although Chromium isotope data gives the most robust indication of extraterrestrial origin, anomalous Iridium and Platinum group element content also indicate an extraterrestrial origin (Alvarez et al 1980, Kyte et al. 2003). It has also been suggested that mineral replacement over billions of years may erase any sign of extraterrestrial material originally present in the spherule layer (Simonson and Glass 2004). For this reason it is possible to confirm a layer’s extraterrestrial origin but it is often impossible to rule out such an origin. In the case of Chicxulub, at locations where ejecta containing melt droplets and the ejecta composed of vapor condensate spherules are both present, the two species are stratigraphically distinct, making a distinction between vapor condensate layers and melt droplet layers by anomalous Iridium possible. Due to redeposition by surface processes, it is possible that other layers will be composed of a mix of melt droplets and vapor condensate spherules.

In addition to impactor size, the impact velocity is computed from the average spherule size using the model of Johnson and Melosh (2012a). This method is described in the Figure 4.1. The average estimated impact velocity from all the known spherule layers is $\sim 21.8 \pm 2.2$ km/s, close to the expected average of $\sim 20.3$ km/s (Minton and Malhotra 2010). The consistency of our impact velocity estimates with the expected average is another indication that the layers we include are indeed vapor condensate spherule layers. We expect that if the layers were composed of melt droplets, which are made by a
completely different process and can be much larger than vapor condensate spherules, our velocity estimates would deviate significantly from this average.

The data from Table 4.1 allows us to construct an impactor Size Frequency Distribution (SFD) for the Earth (Figure 4.2). We expect that the Earth’s impactor SFD obtained from spherule layers should exhibit a power law dependence similar to the impactor SFDs obtained from direct astronomical observations of near-Earth asteroids. Comparing the form of the different impactor SFDs in Figure 4.2, we see an obvious deficit of impactors smaller than ~20 km in diameter in the impactor SFD obtained from spherule layer data. It is plausible that this rollover at smaller impactor sizes is due to either observational or preservation biases. As an impacting body becomes smaller, it creates progressively thinner and sparser layers that are more difficult to recognize and more easily obscured or destroyed by subsequent geologic processes or diluted during initial emplacement (Simonson and Glass 2004). In addition to a bias in favor of thicker layers, the history of large impacts on Earth provided by spherule layers is probably incomplete, as only two regions have been systematically searched for Precambrian spherule layers, the Pilbara Craton in Western Australia (especially the Warrawoona and Hamersley successions) and the Kaapvaal Craton in South Africa (especially the Barberton Greenstone Belt and Griqualand West succession). It is thus not surprising that most of the known layers were discovered in these two regions. These two regions represent strata from 2.63-2.49 Gyr and 3.47-3.24 Gyr. These strata thus represent approximately 10 percent of the Earth’s Impact history over 3.5 Gyr. Considering the poor sampling of much of the geologic record, it is likely that many more spherule layers are yet to be discovered. Additionally,
a preliminary report shows evidence of three more spherule layers in the Barberton Greenstone Belt (Lowe and Byerly 2010).

During the Late Heavy Bombardment (LHB), 4.1-3.8 Gyr, the impactor flux was much higher than the present-day flux (Gomes et al. 2005). It is debated whether the post LHB impactor flux dropped quickly to present-day values or slowly decreased as implied by a solar system model that includes an extended asteroid belt (Bottke et al. 2012). The impactor SFDs inferred from observations of near Earth asteroids represent the expected impactor SFD on Earth assuming that the impactor flux has remained constant over the last 3.5 Gyr, consistent with a quick decrease in post LHB impactor flux. The impactor SFD implied by spherule layers makes no assumption about the time dependence of the impactor flux and therefore, if complete, represents the average impactor flux over 3.5 Gyr. The spherule record represents only ~10% of the total 3.5 Gyr history. Thus, if the impactor flux implied by spherules has remained constant over 3.5 Gyr, we must multiply the current number of impacts by a factor of ~10. This SFD would then disagree with even the highest estimates of current-day impactor flux. A constant impactor flux therefore cannot be simultaneously consistent with spherule layer data and observations of NEAs. This implies the impactor flux was significantly higher 3.5-2.5 Gyr ago, consistent with a gradual decline of the post LHB impactor flux. However, the spherule record cannot rule out other explanations for the heightened impactor flux including the unlikely occurrence of one or more large spikes in the impactor flux that happen to coincide with the two time frames for which there are well-preserved strata. To make a more robust and quantitative conclusion about the time dependence of the post LHB
impactor flux, a more complete search for spherule layers in the geologic record is required.
The Earth’s impactor SFD is plotted as the cumulative number of impacts larger than a given diameter as a function of diameter. The points with vertical black error bars (s.d.) represent the SFD based on spherule layer data from Table 4.1, where impactor diameter is reported as a size range. Each black dot represents a single impact and is plotted at the geometric mean of this size range and the horizontal red error bars are plotted to represent the entire impactor size range. The squares, solid curve, and circles, represent three separate estimates of the Earth’s cumulative impactor SFD obtained by multiplying the present-day impactor flux reported as probability of impacts per year by the time interval of 3.5 Gyr, which is approximately the age of bed S1. The squares are from direct observations of Near Earth Asteroids (NEA)s (Stuart and Binzel 2004). The solid curve is obtained by scaling the SFD of the main asteroid belt to observations of NEAs at smaller sizes where there are many more objects and therefore much less statistical error (Ivanov and Hartmann 2007). The circles are obtained by scaling the SFD of Mars crossing asteroids to observations of NEAs in a similar manner to reference number two (Le Feuvre and Wieczorek 2011). When “multiple layers” are believed to come from the same impact, we assume they do. The red error bar then represents the range from the smallest size indicated by the “multiple layers” to the largest size. For example, we assume that the two spherule beds Jeerinah, and Monteville were created by a single impactor which may be anywhere from 6.3 – 46 km in diameter. The large size range for this particular impact may indicate that one of these layers is from a separate impact or represents a melt droplet layer.

Figure 4.2 The Earth's Impactor Size Frequency Distribution
CHAPTER 5. FORMATION OF MELT DROPLETS, MELT FRAGMENTS, AND ACCRETIONARY IMPACT LAPILLI DURING A HYPERVELOCITY IMPACT


We present a model that describes the formation of melt droplets, melt fragments, and accretionary impact lapilli during a hypervelocity impact. Using the iSALE hydrocode, coupled to the ANEOS equation of state for silica, we create high-resolution two-dimensional impact models to track the motion of impact ejecta. We then estimate the size of the ejecta products using simple analytical expressions and information derived from our hydrocode models. Ultimately, our model makes predictions of how the size of the ejecta products depends on impactor size, impact velocity, and ejection velocity. In general, we find that larger impactor sizes result in larger ejecta products and higher ejection velocities result in smaller ejecta product sizes. We find that a 10 km diameter impactor striking at a velocity of 20 km/s creates millimeter scale melt droplets comparable to the melt droplets found in the Chicxulub ejecta curtain layer. Our model also predicts that melt droplets, melt fragments, and accretionary impact lapilli should be
found together in well preserved ejecta curtain layers and that all three ejecta products can form even on airless bodies that lack significant volatile content. This prediction agrees with observations of ejecta from the Sudbury and Chicxulub impacts as well as the presence of accretionary impact lapilli in lunar breccia.

5.1 Introduction

Ejecta curtain layers found in the geologic record are composed of melt droplets, melt fragments, accretionary impact lapilli, and solid ejecta (Schulte et al. 2010). As the title of this paper implies, the focus of this work is the formation of melt droplets, melt fragments, and accretionary impact lapilli, which we will refer to as ejecta products. A comprehensive model describing the formation of these ejecta products coupled with geologic observations of ejecta curtain layers may allow us to infer the properties of the impacting body that created these layers. This would yield valuable information about the Earth's impact bombardment history even when a source crater cannot be found. Any information about the Earth's bombardment history is especially valuable because impact craters on Earth are quickly obscured or destroyed by surface weathering and tectonic processes (Simonson and Glass 2004). Although global fireball layers have been used to estimate Earth's bombardment history (Johnson and Melosh 2012b), only about half of the known ejecta layers are global deposits while the remainder of the layers appear to be more proximal ejecta curtain layers (Glass and Simonson 2012). It is apparent that understanding the formation of melt droplets, melt fragments, accretionary impact lapilli, and ejecta curtain layers is imperative.
The basic process of impact cratering is understood reasonably well (Melosh 1989). When an impactor hits the Earth, or other target, a shock wave passes through the impactor, which is decelerated, compressed, and heated. At the same time, a shock wave moves through the target accelerating and heating it. After passage of the shock wave, accelerated material moves away from the point of impact creating a crater. This flow of material is called the excavation flow. When the excavation flow emerges above the surface, it ejects material ballistically, producing an expanding cone of material called the ejecta curtain. Although most of the excavated mass is ejected at low velocities and lands just outside the crater rim, a small fraction of excavated material is ejected at high velocity and for Chicxulub and similar large craters this material can be found thousands of kilometers from the point of impact (Smit 1999).

After final emplacement, the ejecta form a layer that can be found in the geologic record (Smit 1999). Because there is no universally accepted terminology that distinguishes this layer from the global fireball layer, we here introduce the term “ejecta curtain layer” for this layer of material, which was ejected as part of the excavation flow. One of the best-studied ejecta curtain layers was deposited by the Chicxulub impact (Smit 1999), which formed when a roughly 10 km diameter impactor struck the Earth 66 Myr ago (Alvarez et al. 1980). This layer extends a few thousand kilometers from the point of impact but the thickness of the ejecta curtain layer decreases rapidly as the distance from the point of impact increases (Schulte et al. 2010). The ejecta products also become smaller as the distance from the point of impact increases (Schulte et al. 2003).
In addition to the Chicxulub ejecta curtain layer there is also a much thinner global ejecta layer, which forms the globally recognized K-Pg boundary layer (Smit 1999, Schulte et al. 2010). This layer, which lies atop the ejecta curtain layer, is only ~3mm thick and is composed of closely packed ~250 micron diameter vapor condensate spherules (Smit 1999). The layer also contains the extraterrestrial signature of the impactor, most readily indicated by a large Iridium anomaly (Shulte et al. 2010). For typical impact velocities of ~20 km/s on Earth, the impactor and a roughly equal mass of target material are shocked to high levels and come to the liquid vapor coexistence curve from the vapor side (Figure 5.1). This material is highly energetic and expands enormously during adiabatic release. During this expansion, the material decouples from the excavation flow, forming a vapor plume or fireball (Figure 5.2). When this material cools and reaches the liquid-vapor coexistence curve, molten spherules condense from the vapor (Johnson and Melosh 2012a). For impactors larger than ~10 km in diameter, such as the Chicxulub impactor, the spherules fall in a layer that covers the entire globe (Johnson and Melosh 2012b). In this paper we will consistently refer to these global ejecta layers, composed of vapor condensate spherules, as global fireball layers.
Figure 5.1 Release Adiabats and Liquid Vapor Coexistence Curve.

Thermodynamic paths of the adiabatic release of shocked SiO\textsubscript{2} from high pressure are plotted on a log Pressure versus Temperature diagram. The Hugoniot curve, indicating the final result of increasingly strong shock compression of quartz, is shown as a heavy line, while the thin colored lines are decompression adiabats. The liquid/vapor coexistence curve separating liquid and vapor phases is shown as a heavy line and the critical point by a heavy dot. The numbers labeling the release adiabats are the particle velocities in the shocked material in km/s. These velocities can be interpreted as the outcome of an impact experiment between identical materials at twice the particle velocity. Thus, the curve labeled 7 is the release adiabat of a face-on impact between two quartz plates at 14 km/s. Material described by the blue adiabats decompresses and forms a boiling liquid when it reaches the coexistence curve creating melt droplets. The red adiabats are so strongly shocked that when they decompress they form a vapor that then condenses into spherules when the adiabat reaches the coexistence curve (After Johnson and Melosh 2012 a).
Figure 5.2 Impact Time Series

Plots showing the position of material during the initial stages of a 10 km diameter silica ($\text{SiO}_2$) impactor striking a silica target at 13 km/s (left column) and 20 km/s (right column). The origin marks the point of impact. Material to the left of the origin is colored according to its temperature while material to the right of the origin is colored according to its density. The color bars do not encompass the full range of densities and temperature, only an illustrative sub-set. iSALE model input parameters are described in Table 5.1.
Table 5.1 iSALE Input Parameters (Barringer Release)

<table>
<thead>
<tr>
<th>Parameter Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of high resolution cells in x-direction</td>
<td>800</td>
</tr>
<tr>
<td>Number of high resolution cells in y-direction</td>
<td>1200</td>
</tr>
<tr>
<td>Cell size in x-direction</td>
<td>25 m</td>
</tr>
<tr>
<td>Cell size in y-direction</td>
<td>25 m</td>
</tr>
<tr>
<td>Surface temperature</td>
<td>273 K</td>
</tr>
<tr>
<td>Gravitational acceleration</td>
<td>9.81 m/s²</td>
</tr>
<tr>
<td>Projectile diameter</td>
<td>10 km</td>
</tr>
<tr>
<td>Projectile material type</td>
<td>Silica</td>
</tr>
<tr>
<td>Target material type</td>
<td>Silica</td>
</tr>
<tr>
<td>Projectile strength</td>
<td>None</td>
</tr>
<tr>
<td>Target strength</td>
<td>None</td>
</tr>
</tbody>
</table>

For the purposes of this paper, we make a clear distinction between the normal ejecta layer and the global fireball layer, but this distinction may not be clear for most layers found in the geologic record. The Sudbury ejecta layer is one example, which does not have a clear distinction between a fireball layer and a normal ejecta layer. This ambiguity is likely the result of the mixing of fireball and normal ejecta material during deposition of the layer (Cannon et al. 2010). As previously stated, these ejecta curtain layers are composed of solid rock fragments, melt droplets, melt fragments, and accretionary impact lapilli and lack significant projectile contamination when they can be distinguished from the global fireball layer (Schulte et al. 2010). Although cold solid rock fragments make up a large portion of the ejecta curtain, models for the formation and sizes of cold solid rock fragments are beyond the scope of this paper and may be the subject of future work. Here we focus on the formation of melt droplets, melt fragments and accretionary impact lapilli, which we will describe in turn.
Melt droplets are previously molten droplets that form when material reaches the liquid vapor coexistence curve from the liquid side (Figure 5.1). We make a distinction between vapor condensate spherules and melt droplet spherules because we believe they form in very different ways (Figure 5.1). However, it is not always possible to determine which of the two types a given spherule is in the geologic record. The presence of lechatelierite, clear silica glass formed by melting of relict quartz grains likely indicate the spherules are melt droplets, not vapor condensates (Glass and Simonson 2012). However, the primary compositions of many spherules have been completely replaced by other minerals making this distinction difficult or impossible (Glass and Simonson 2012). Most melt droplets are mm scale and spherical but they can be teardrop and dumbbell shaped. These rotational forms indicate that interaction between molten drops and ambient vapor play an important role in their formation (Elkins-Tanton et al. 2003).

Melt fragments are rarer and are usually larger than a centimeter in size. Melt fragments are sometimes called melt clasts or tektites although the term tektite is more specific and refers to a glassy melt fragment that is geochemically and isotopically similar to the terrestrial upper crust (Koeberl 1986). Melt fragments take on rotational forms similar to melt droplets. Although melt fragments and melt droplets differ in size, there is not always a clear dividing line between the two. Here, we argue that melt droplets are the result of the break up of larger melt fragments. Thus, one might naturally expect a continuum of particle sizes between the melt droplets and melt fragments. Some observations of Chicxulub and Sudbury ejecta indicate a continuum of particle sizes exist (Schulte et al. 2003, Cannon et al. 2010), while other observations of the Sudbury ejecta
seem to indicate melt droplets and melt fragments represent two distinct populations (Pufahl et al. 2007). The work of Cannon et al. (2010), which covers many Sudbury ejecta locations, showed that the difference between these observations is likely caused by differences in the depositional environments studied.

Accretionary impact lapilli are roughly spherical particles composed of accreted fine-grained material. Although they may form through the agency of molten silicate, not water, accretionary impact lapilli are morphologically similar to volcanic accretionary lapilli. The term lapillus is traditionally a size classification but accretionary impact lapilli range in size from larger than a centimeter to smaller than a millimeter. Accretionary impact lapilli may not be found in all ejecta curtain layers as these aggregates, if similar to volcanic accretionary lapilli, can be quite delicate, disintegrating on impact (Walker 1981). Note that some volcanic accretionary lapilli appear to be quite robust, surviving transport by flowing water (Lowe 1999). These differences likely depend on the details of the formation and deposition of these different accretionary lapilli.

The problem of ejecta product formation is not new and there have been several past attempts to describe the formation of ejecta curtain products. In 1991, Melosh and Vickery explored melt droplet and melt fragment formation, modeling the melt ejection as a half sphere expanding into free space. We find this geometry more closely represents the geometry of the vapor plume, while the melt is actually ejected as part of the ejecta curtain and represents a significantly different geometry (Figure 5.2). Several authors
describe the formation of accretionary impact lapilli as a process that takes place in turbulent density currents, similar to the formation of volcanic lapilli (Branney and Brown 2011, Knauth et al. 2005, McKay and Morrison 1971). This description is problematic, because lapilli are found on the moon (McKay and Morrison 1971). On the moon, without an atmosphere or non-condensable entrained vapor, turbulent density currents should not form (Wilson 2009). The formation of lapilli on the moon is also hard to explain because lapilli require the presence of liquid to bind the fine-grained material and the moon arguably lacks significant volatile content (Gilbert and Lane 1994, Saal et al. 2008). In our model accretionary impact lapilli form during the ejection process and we argue that molten silicate acts as the binding agent, although any condensable material in the ejecta curtain could act as the binding agent. Thus, we expect accretionary impact lapilli can form on any rocky body, even those that contain no water and have no atmosphere.

In this paper, we introduce a model of ejecta product formation within the ejecta curtain early in the ejection process, well before re-entry into an atmosphere or ballistic emplacement. Our model makes order of magnitude estimates of the size of melt droplets and melt fragments that are in agreement with observations of Chicxulub and Sudbury ejecta. Our work also predicts that mm scale melt droplets should be found along with accretionary impact lapilli and the rarer melt fragments. This prediction is consistent with the observation of melt droplets and accretionary impact lapilli found together in both the Chicxulub ejecta ~2500 km from the point of impact (Yancey and Guillemette 2008) and the Sudbury ejecta found ~800 km from the point of impact (Addison et al. 2005).
5.2 Results

In Section 5.2.1 we use iSALE to create high-resolution hydrocode models of the ejecta curtain. We use these models to develop an understanding of aspects of the ejecta curtain that are important to our model of ejecta product formation. This includes an understanding of what material represents melt/solid and where this material comes from. Figure 5.3 is a schematic model of the ejecta curtain and the processes that create ejecta products. When material comes to the liquid-vapor coexistence curve from the liquid side (Figure 5.1) the expanding fluid forms a boiling liquid with an average fragment size that depends on the strain rate. Some of these large melt fragments may avoid further fragmentation, retaining their large sizes (Section 5.2.2). Although Figure 5.3 shows melt fragments forming in the ejecta curtain, they actually form below the pre-impact surface. As the fragmented mixture of vapor and melt is accelerated by gas pressure gradients, gas drag from the impact vapor causes these melt fragments to break up into smaller millimeter scale melt droplets (Section 5.2.3). After the material is ejected ballistically, turbulence in the ejecta curtain causes accretionary impact lapilli to grow as they accrete a mixture of fine-grained solid fragments and melted material (Section 5.2.4).
A schematic illustration of the ejecta curtain and the processes that form the ejecta products within it. The gray represents fragmented solid material. The dark orange represents melted material. In reality distinction between melted and un-melted material will be less clear because some material will be partially melted. The material in the ejecta curtain is textured to illustrate that it is made up of small particles of melted or solid material with void space or vapor making up a significant volume fraction. The circles with arrows represent the largest turbulent eddies that can form in the ejecta curtain. The large blocks on the underside of the ejecta curtain represent spall fragments. **Frame a** describes the process that forms melt fragments. At $t_1$, a supercritical fluid is about to reach the liquid-vapor coexistence curve from the liquid side. Upon reaching the coexistence curve, at $t_2$, this expanding fluid fragments, forming a boiling liquid with liquid fragments whose size depends on the strain rate at the time of fragmentation. **Frame b** shows the process that creates melt droplets in two different time steps. At $t_1$, aerodynamic forces are deforming the droplet from its spherical equilibrium shape. At $t_2$, the relative velocity of the vapor is larger and the aerodynamic forces on the droplet exceed the forces of surface tension causing the droplet to break up into several smaller droplets. **Frame c** shows the process that creates accretionary impact lapilli. Accretionary impact lapilli grow by accreting melt droplets and/or small shards of rock that are coated in liquid by vapor condensation or collisions with melt droplets. The large lapilli collide with the smaller particles at a relative velocity $V$ that is determined by the turbulent velocity.
5.2.1 Detailed Model of the Ejecta Curtain

To better understand the properties of the ejecta curtain, we performed impact simulations using the axisymmetric finite-difference 2-D hydrodynamics code iSALE. The iSALE shock hydrodynamics code (Wunnemann et al., 2006) is an extension of the SALE code (Amsden, 1980). SALE was built to model hypervelocity impact processes in solid materials, and iSALE extends this work to include sophisticated constitutive models, equations of state, and to account for multiple materials. For a description of our model input parameters see Table 5.1.

All of our simulations use a 10 km diameter impactor that roughly corresponds to the size of the impactors that created the Chicxulub and Sudbury impact structures assuming a 20 km/s impact velocity typical for asteroids impacting the Earth (Collins et al. 2008a, Grieve and Therriault 2000, Minton and Malhotra 2010). Ignoring possible atmospheric effects, the choice of impactor size is not important because, as we describe in Appendix B.1, we can scale our results to other impactor sizes using arguments based on hydrodynamic similarity. To reduce computational expense, our models are completely hydrodynamic and do not include a strength model. The high velocity material we focus on originates from a region that is very close to the point of impact. This material should be completely fractured and has ejection velocities higher than 1 km/s, so the inclusion of a strength model would have a minimal effect on this material.
Although it is not the most realistic choice, we assume that the impactor and target are made of SiO$_2$. We make this choice so we can use the ANEOS equation of state (EOS) for silica, which accounts for the dissociation of molecules at high temperatures (Melosh 2007). Experiments show that this EOS describes the liquid vapor coexistence curve well (Kraus et al. 2012). Although the ANEOS EOS for silica is arguably the most accurate EOS describing the shock physics of geologic material, experiments done by Kurosawa et al. (2012) and Kraus et al. (2012) show that ANEOS for silica does a poor job at estimating the entropy on the Hugoniot. Kraus et al. (2012) find that melting and vaporization occurs at 47 GPa and 75 GPa respectively, somewhat lower than the 65 GPa and 95 GPa estimated by the ANEOS EOS (Melosh 2007). We do not make a distinction between incipient melting and complete melting because the ANEOS EOS for silica does not include the latent heat of melting (Melosh 2007). It is obvious that that there is room for significant improvement of EOSs for geologic materials used in shock physics codes.

Figure 5.2 shows the first stages of two impacts with impact velocities of 13 km/s and 20 km/s. We use an impact velocity of 13 km/s because it is the highest impact velocity where no vapor plume develops. Even after 40s there is no vapor plume present in the model with an impact velocity of 13 km/s. Considering the work of Kraus et al. (2012) and Kurosawa et al. (2012) a vapor plume would probably develop at velocities lower than the 13 km/s if a more realistic equation of state were used. The other impact velocity we use is 20 km/s. We choose this velocity because, in addition to clearly showing a vapor plume, 20 km/s is close to the expected average asteroid impact velocity on Earth (Minton and Malhotra 2010). Figure 5.4 shows that material that comes to the liquid
vapor coexistence curve from the vapor side (red lines Figure 5.1 and Figure 5.4) expands more during adiabatic release than material that comes to the coexistence curve from the liquid side (blue lines Figure 5.1 and Figure 5.4).

Figure 5.4 provides a qualitative explanation for what happens in Figure 5.2. At an impact velocity of 13 km/s even the most highly shocked material comes to the liquid vapor coexistence curve from the liquid side and little expansion occurs during adiabatic release from the Hugoniot. Thus, the material stays coupled to the excavation flow and forms part of the ejecta curtain, which is eventually deposited as an ejecta curtain layer (Figure 5.2 left column). At an impact velocity of 20 km/s some material comes to the coexistence curve from the vapor side after undergoing significant expansion during adiabatic release from the Hugoniot. This expansion causes the material to decouple from the excavation flow, forming a vapor plume (Figure 5.2 right column). Thus, at an impact velocity around 20 km/s, typical for asteroids impacting Earth, both an ejecta curtain and a vapor plume form. This ultimately results in the formation of both an ejecta curtain layer and a global fireball layer, and thus naturally accounts for the double layer structure of the K/Pg ejecta deposits found up to 5000 km from the impact site (Schulte et al. 2010).
Figure 5.4 Density Change During Release

Ratio of density on the Hugoniot curve (Figure 1) to density on the liquid-vapor coexistence curve (Figure 1) assuming adiabatic expansion plotted as a function of peak shock pressure. The blue curve represents material that comes to the liquid-vapor coexistence curve from the liquid side. The red curve represents material that comes to the liquid-vapor coexistence curve from the vapor side. The large black dot represents material that comes to the liquid-vapor coexistence curve at the critical point; this material has a peak shock pressure of 315 GPa and a peak density 6000 kg/m$^3$ and unloads to a critical density 549 kg/m$^3$. The dashed line acts as a guide to the eye to show the most highly shocked material created by a 13 km/s impact, this material has a peak shock pressure of 213 GPa. The solid line acts as a guide to the eye to show the most highly shocked material created by a 20 km/s impact, this material has a peak shock pressure of 452 GPa. The black curve represents material that is melted but does not separate into a 2-phase mixture upon release. The gray curve represents solid material. The triangle represents the shock pressures of 65 GPa required to melt material. The square represent the shock pressure of 95 GPa above which material will form a 2-phase mixture upon release to a pressure of 1 bar.
Figure 5.5 shows that highly shocked material coming from depth is located on the side of the ejecta curtain nearest the point of impact, while material that experiences lower peak shock pressures originates near the surface and is located on the leading edge of the ejecta curtain. Figure 5.6 shows that distant parts of the ejecta curtain move at higher velocities than portions that are closer to the point of impact. This velocity structure is expected for the ejecta curtain and is consistent with material in ballistic flight. Figure 5.6 also shows that 3.0 s after impact, material ejected at velocities greater than ~1400 m/s is in ballistic flight. After 3.0s material with lower velocities will also be ballistically ejected. Thus, the choice to focus on material ejected at velocities higher than 1400 m/s, corresponding to a range of ~200 km on Earth, is made simply to limit computational expense. Our models have a relatively high resolution of 200 cells per projectile radius (cppr), and can resolve material ejected at velocities as high as ~5.9 km/s for the 13 km/s impact velocity and ~6.8 km/s for the 20 km/s impact velocity. These ejection velocities do not represent a physical limit on the ejection velocity they only reflect what can be resolved by the code. Furthermore, a small amount of material is jetted during an actual impact and will have ejection velocities higher than the impact velocity (Melosh 1989).
Position of Lagrangian tracers 3.0 s after a 10 km diameter impactor struck the target at 13 km/s (left) and 20 km/s (right). The tracers are colored according to the highest pressure that the tracers have experienced (peak shock pressure). The size of the markers is apparent in the right figure. The plotted tracers are from both the projectile and the target. The most highly shocked tracers roughly track the projectile target interface. Note that in the figure, the markers of tracers with higher peak shock pressure are printed on top of tracers with lower peak shock pressures. Meaning that if two tracers were plotted at the exact same position the tracer with a lower peak shock pressure would not appear on the plot.
Figure 5.6 Ejection Velocity

Position of Lagrangian tracers 3.0 s after a 10 km diameter impactor struck the target at 13 km/s (left) and 20 km/s (right). The tracers are colored according to the magnitude of their ejection velocities. All of the tracers in these plots represent target material in agreement with observations showing the ejecta curtain layers are composed primarily of target material. Note that in the figure, the markers of tracers with higher ejection velocities are printed on top of tracers with lower ejection velocities. Meaning that if two tracers were plotted at the exact same position the tracer with a lower ejection velocity would not appear on the plot.

The peak shock pressure and the ejection velocity, defined as the magnitude of tracer velocities 3 seconds after the impact, are plotted in Figure 5.7. These plots represent all of the tracers shown in Figure 5.6 that have an ejection velocity greater than 1400 m/s. For the 20 km/s impact this includes some highly shocked material that will actually be part of the vapor plume not the ejecta curtain. We choose to include this material because the true distinction between the vapor plume and the ejecta curtain is unclear. However, as Figure 5.7 shows, the mass of highly shocked material that will actually be part of the vapor plume is much less than the mass of material in the ejecta curtain ejected at these velocities. Thus, our choice to avoid making an arbitrary distinction between the vapor
plume and ejecta curtain and include some vapor plume material does not significantly affect our results.

The black curve in Figure 5.7 is the Hugoniot plotted as peak particle velocity as a function of peak shock pressure. Tracers lying below the black curve represent material that is ejected at a velocity higher than the peak particle velocity expected based on its peak shock pressure and the Hugoniot. This material, called spall, has higher than expected ejection velocities because of the interactions between the shock wave and the rarefaction near the free surface (Melosh 1985). The material above the black curve is sourced from a region further below the free surface where the rarefaction, arriving after the shock wave, tends to decrease the velocity of the material (Melosh 1985). As our schematic (Figure 5.3) illustrates, the spalled material is ejected as part of the ejecta curtain. Contrary to the intuitive idea that material ejected at higher velocities will have a higher average peak shock pressure, Figure 5.7 shows that the average peak shock pressure in the ejecta curtain is not a function of the ejection velocity, at least for material ejected at velocities above 1400 m/s. Similar results for more proximal ejecta were found by Collins et al. (2008b).
Figure 5.7 Peak Shock Pressure versus Ejection Velocity

Tracers (colored dots) are plotted according to their peak shock pressure and ejection velocities 3.0 s after a 10 km diameter silica impactor struck a silica target at 13 km/s (top) and 20 km/s (bottom). Tracers move as Lagrangian particles and approximately track the motion of a parcel of material with a mass determined by the initial spacing and location of the tracers. The tracers are colored according to the mass of material they represent. The blue squares represent the average peak shock pressure by mass in bins with a width of 100 m/s. The black curve represents the peak particle velocity of material shocked to a given peak shock pressure given by the Hugoniot equation. Tracers lying under the black curve represent spall. Note that incipient vaporization occurs at a shock pressure of 95 GPa and melting occurs at shock pressures above 65 GPa.
We calculate the ejecta thickness as a function of distance from the point of impact from our high-resolution model of the ejecta curtain. We again consider material with velocities above 1400 m/s. On Earth this material will land ~200 km and further from the point of impact. For smaller craters this high velocity ejecta will be very distal, but for a large enough crater (larger than ~400 km in diameter) some of this material will actually land within the crater rim. As Figure 5.8 shows, the differential mass of ejecta as a function of ejection velocity is $M(v_{ej}) \propto v_{ej}^{-4.8\pm0.1}$ for a 20 km/s impact velocity. Note that this mass distribution is not a cumulative distribution, which is given by $M_{cum}(v_{ej}) \propto v_{ej}^{-3.8\pm0.1}$ and reports all of the mass with velocities greater than $v_{ej}$. Figure 5.8 also shows that the velocity dependence for $M(v_{ej})$ does not depend on our model resolution. The conservation of mass requires that $M(v_{ej}) = 2\pi\rho D \Delta r t$, where the $D$ is the average distance from the point of impact that the ejecta travels, $\Delta r$ is the difference between the maximum range and minimum range that a portion of the ejecta curtain with velocities ranging from $v_{ej} - \Delta v/2$ to $v_{ej} + \Delta v/2$ will have, and $t$ is the thickness of the ejecta at a given range. Ignoring the curvature of the planet, and assuming a constant ejection angle, we find $D \propto v_{ej}^2$ and $\Delta r \propto v_{ej}$. Then for a constant $\Delta v$ and $v_{ej} \geq 1400$ m/s, as in Figure 5.8, we find

$$t \propto v_{ej}^{-7.8\pm0.1} \propto D^{-3.9\pm0.05}.$$ (5.1)

We find that including the ejection angle still leads to $t \propto D^{-3.9\pm0.05}$ and Figure 5.8 suggests that this expression does not depend on impact velocity. This thickness dependence for distal ejecta is consistent with $t \propto D^{-4.4\pm0.3}$ observed for the Australasian tektite strewn field (Glass and Pizzuto 1994).
Figure 5.8 Mass Ejected versus Ejection Velocity

Histogram of mass as a function of ejection velocity 3.0 s after a 10 km diameter silica impactor struck a silica target at 13 km/s (left) and 20 km/s (right). The Lagrangian tracers approximately track the motion of a parcel of material with a mass determined by the initial spacing and location of the tracers. Thus, the marks denote the mass of tracers in bins with a width of 100 m/s. The right figure also shows the histogram plotted for resolutions of 25, 50, and 100 cells per projectile radius (cppr). The resolutions correspond to a maximum ejection velocity of 2.40 km/s, 3.10 km/s, and 4.22 km/s respectively. The black dashed line is the best linear fit to the 200 cppr data between 1500 and 3600 m/s. This fit implies that $M(v_{ej}) \propto v_{ej}^{-5.0\pm0.1}$ for the 13 km/s impact velocity (left) and $M(v_{ej}) \propto v_{ej}^{-4.8\pm0.1}$ for the 20 km/s impact velocity (right). A comparison of the different resolution data shows agreement at lower velocities where the ejected material is well resolved.

Our calculated dependence of ejecta thickness as a function of range is significantly different from the often-used $t \propto D^{-3.0}$ of McGetchin et al. (1973). Our $t \propto D^{-3.9\pm0.05}$ dependence is also steeper than the dependence derived by Housen et al. (1983), which
gives $t \propto D^{-2.75 \pm 0.25}$ for the full theoretical range of target strength. However, Housen et al. (1983) point out that their power-law may not hold for high-velocity ejecta sourced from a region near the impact, where energy and momentum coupling occurs and the point source approximation is expected to fail. As Figure 5.9 shows, most of the high velocity ejecta comes from a region close to the point of impact. To test our results, we also made calculations using a different equation of state. Using the Tillotson EOS for aluminum (Tillotson 1962) we modeled a 10 km diameter aluminum impactor impacting an aluminum target at 20 km/s and found the same $t \propto D^{-3.9 \pm 0.05}$ dependence. Our $t \propto D^{-3.9 \pm 0.05}$ dependence is also consistent with hydrocode simulations by Shuvalov (2011), which show a similar departure from the McGetchin et al. (1973) and Housen et al. (1983) power laws for high velocity ejecta. Note that the Shuvalov’s (2011) simulations show the expected $t \propto D^{-3.0}$ for the low velocity ejecta of smaller craters. This result implies that less high velocity material is ejected by hypervelocity impacts than previously thought.
Figure 5.9 Provenance Map of Ejection Velocity

Provenance map showing the position of Lagrangian tracers before a 10 km diameter impactor strikes the target at 13 km/s (top) and 20 km/s (bottom). The tracers are colored according to their ejection velocities 3.0 s after impact. All of the tracers in these plots represent target material in agreement with observations showing the ejecta curtain layers are composed primarily of target material.
5.2.2 Melt Fragments

When highly shocked material reaches the liquid-vapor coexistence curve from the liquid side the expanding fluid fragments, forming a boiling liquid (Figure 5.1, Figure 5.3 a). Grady (1982) finds that the balance between the surface tension, $\sigma$, and relative kinetic energy of these fragments determines the diameter of melt fragments, $d_0$. This balance gives

$$d_0 = \left(\frac{40\sigma}{\rho \varepsilon^3}\right)^{\frac{1}{3}}$$  \hspace{1cm} (5.2)

where $\rho \approx 2500$ kg/m$^3$ is the density of the liquid and $\varepsilon = -\dot{\rho}/(3\rho)$, which is the linear strain rate assuming an isotropic expansion. Although $\sigma$ is temperature dependent and $\sigma = 0$ at the critical point, for a wide range of temperatures liquid silica has a $\sigma \approx 0.3$ N/m (Boča et al. 2003). We assume that $\dot{\varepsilon} \approx v_{ej}/R_f$, where $v_{ej}$ is the ejection velocity and $R_f$ is the radial distance from the point of impact where fragmentation takes place. Note that we prefer to use this rough estimate of strain rate, rather than calculating it directly from the hydrocode because we wish to display the dependence of fragment size on impact parameters explicitly, in a way not tied to a particular code calculation. More detailed analysis shows that this estimate for strain rate only changes the estimated fragment size by a factor of order unity. Using the tracer data to estimate $v_{ej}$ and $R_f$, as described in Appendix B.2, we can estimate the size of melt fragments as a function of the ejection velocity using equation 5.2 (Figure 5.10). Using the power law fit from Figure 5.10 and hydrodynamic scaling we can derive the following equation for the size of melt fragments as a function of ejection velocity, impact velocity, and impactor size.
\[ d_0 \approx 0.14 \left( \frac{v_{ej}}{V_{imp}} \right)^{-0.81\pm0.015} \left( \frac{R_{imp}}{V_{imp}} \right)^{2/3} \text{ SI units (5.3)} \]

An impactor that is 1 km in diameter creates melt fragments that are \(~1/5\) the size reported in Figure 5.10 or \(~4-8\) cm in diameter. These sizes are more consistent with observed sizes of tektites and melt fragments than the 20-40 cm size estimates for the 10 km diameter impactor (Montanari and Koeberl 2000, Simonson and Glass 2004). It is possible that the size of melt fragments created by large impacts is reduced by some other process, e.g., the fragments may break up as they mutually collide, break up because of interactions with the surrounding vapor, ablate during re-entry into the Earth’s atmosphere (Melosh and Vickery 1991), fragment when the solid melt fragments impact the Earth’s surface, or fragment through thermal stresses induced when melt fragments land in water (Glass et al. 1997).
Figure 5.10 Melt Fragment Size as a Function of Ejection Velocity

The '+' signs represent size estimates made using equation 5.2 and tracer data for the 10 km diameter impactor and a 20 km/s impact velocity (Appendix B.2). The solid line is the best power-law fit to the tracer output. The uncertainty in the exponent, reported in the legend, is the two-sigma confidence bound to our fit.

In 2003 Elkins-Tanton et al. provided a laboratory model for the formation of “splash-form” tektites, which focuses on the shape of tektites. This study concluded that tektites larger than 3mm in size could not be molten during re-entry into the Earth’s atmosphere. Also, any tektite that takes the form of a body of revolution, requiring its rotational velocity to be greater than 1% of its relative translational-velocity, has an estimated maximum size of ~8 cm. Although there is no reason to assume that melt fragments will have rotational velocities that are greater than 1% of their translational velocities, most melt fragments and tektites assume shapes of bodies of rotation (Elkins-Tanton et al. 2003). This ~8 cm size limit may explain why our size estimates for a 10 km diameter impactor are substantially larger than observed melt fragment sizes.
In the next section, we argue that interactions with the surrounding vapor cause most, but not all, melt fragments to break up into smaller melt droplets. Thus, we expect that completely melted material that has not reached the point of incipient vaporization will yield melt fragments that are more likely to retain their initially large sizes. This relatively lightly shocked material comes from near the surface. This conclusion that the largest melt fragments will be composed of near surface target material is consistent with the isotopic and geochemical composition of tektites (Montanari and Koeberl 2000).

5.2.3 Melt Droplets

The mechanism of melt droplet formation described in this section is very similar to the mechanism described by Melosh and Vickery (1991). In this model, we use a more realistic geometry to represent the excavation flow, whereas Melosh and Vickery (1991) modeled melt droplet formation in an expanding hemisphere, a geometry that more closely resembles the vapor plume.

Following the initial fragmentation of the supercritical fluid into vapor and liquid, this two-phase mixture continues to accelerate before it is ballistically ejected. Once fragmentation occurs, melt can only be accelerated by aerodynamic drag as the surrounding vapor flows past the melt. The balance of the aerodynamic drag force and surface tension ultimately determines the size of the melt droplets. When the Weber number defined as $We = \rho (v_v - v_d)^2 d / \sigma$, surpasses a critical value, $We_c \sim 14$ (Wierzba...
1990), the melt droplets will break up as shown in Figure 5.3 b. Thus, the maximum melt droplet size is given by

$$d_m = \frac{\sigma}{\rho_v(v_v - v_d)^2}$$  \hspace{1cm} (5.4)

where $\sigma \approx 0.3$ N/m is the surface tension of the melt droplets, $\rho_v$ is the density of the vapor and $v_v$ and $v_d$ are the velocity of the vapor and drop respectively. As the vapor streams past the melt droplets aerodynamic drag accelerates the droplets with,

$$\frac{dv_d}{dt} = \frac{3C_d \rho_v (v_v - v_d)^2}{4 \rho_d d_m} = \frac{3C_d \rho_v^2}{4 \rho_v \sigma \rho_d} (v_v - v_d)^4$$  \hspace{1cm} (5.5)

where $C_d \approx 0.5$ is the drag coefficient (Clift et al. 1978) and $\rho_d \approx 2500$ kg/m$^3$ is the droplet density. The second equality assumes that droplets have reached an equilibrium size set by the critical Weber number and that the liquid and vapor have come to a constant differential velocity $\Delta v = v_v - v_d$. When this occurs $\frac{dv_d}{dt} = a$, where $a$ is the bulk acceleration of the two-fluid flow. Using equations 5.4 and 5.5 we solve for the equilibrium size of the melt droplets and find

$$d_m = \sqrt{\frac{3W_e \sigma C_d}{4 \rho_d a}}$$  \hspace{1cm} (5.6)

Using the tracer data to estimate the maximum acceleration $a$ experienced after fragmentation, as described in Appendix B.2, we can estimate the size of melt droplets as a function of the ejection velocity using equation 5.6 (Figure 5.11). Using the power law fit from Figure 5.11 and hydrodynamic scaling we can derive the following equation for the size of melt droplets as a function of ejection velocity, impact velocity, and impactor size.

$$d_m \approx 0.025 \left( \frac{v_{ej}}{V_{imp}} \right)^{-0.97 \pm 0.23} R_{imp}^{\frac{1}{2}} V_{imp}^{-1} \hspace{1cm} \text{SI units}$$  \hspace{1cm} (5.7)
The uncertainty reported in the exponent is only the uncertainty of our power law fit. Indeed, equation 5.7 should only be taken as an order of magnitude estimate. Although there is reason to believe the viscosity of melt droplets is low (below 0.1 Pa s) at the time of fragmentation (Shaw 1972, Elkins-Tanton et al. 2003), if the melt droplets had a viscosity above 1 Pa s the critical weber number could be 3-4 times higher than the value we used (Wierzba 1990). The largest source for uncertainty probably comes from our estimate of acceleration at the time of fragmentation (Appendix B.2). Considering these uncertainties, Figure 5.11 shows that our estimated melt droplet sizes, although about a factor of two too small, are generally in decent agreement with observation of the Chicxulub ejecta (Table 5.2). The derived weak dependence of droplet size on impactor size (equation 5.7) also agrees well with observation because most melt droplets are roughly of mm scale (Simonson and Glass 2004). The scatter of tracer data in Figure 5.11 reflects the variation in acceleration histories that different tracers ejected at the same velocity experience. This variation in acceleration histories leads to a wide dispersion in sizes of melt droplets found at any given site. This agrees well with observation. For example, although the average spherule size in Brazos River, Texas is ~1mm, the maximum spherules size at this location is ~2 mm (Schulte et al. 2003).
Figure 5.11 Melt Droplet Diameter as a Function of Ejection Velocity

The ‘+’ signs represent size estimates made using equation 5.6 and tracer data for the 10 km diameter impactor and a 20 km/s impact velocity (Appendix B.2). The red diamonds represent spherule data taken from Table 5.2. Ejection velocities are calculated using the distance from point of impact and assumes a typical 45 degree ejection angle. The comparison of model estimates and actual spherule data assumes that a roughly 10 km diameter impactor striking with a velocity of 20 km/s formed the Chixculub structure. The solid line is the best power-law fit to the tracer output. The uncertainty in the exponent, reported in the legend, is the two-sigma confidence bound to our fit.
Table 5.2 Observations of Average Spherule Size

Average spherule diameter found in Chicxulub ejecta at several locations and distances from the point of impact (after Schulte et al. (2003)). The distances come from Schulte et al (2010). Much of the spherule data is reported as only an average with no estimate of deviation from the mean or uncertainty.

<table>
<thead>
<tr>
<th>Region</th>
<th>Location/Site</th>
<th>Mean melt droplet size (mm)</th>
<th>Distance from Impact site (km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Belize</td>
<td>Albion Island</td>
<td>3</td>
<td>300</td>
</tr>
<tr>
<td>Haiti</td>
<td>Beloc</td>
<td>1.2</td>
<td>500</td>
</tr>
<tr>
<td>Caribbean Sea</td>
<td>ODP 165</td>
<td>1.5</td>
<td>600</td>
</tr>
<tr>
<td>NE Mexico</td>
<td>El Peñon, La Lajilla, El Mimbral</td>
<td>1.5</td>
<td>700-800</td>
</tr>
<tr>
<td>NE Mexico</td>
<td>La Sierrita</td>
<td>1.2</td>
<td>800</td>
</tr>
<tr>
<td>Alabama</td>
<td>Moscow Landing, Shell Creek</td>
<td>2-3</td>
<td>900</td>
</tr>
<tr>
<td>Texas</td>
<td>Brazos River</td>
<td>1</td>
<td>900</td>
</tr>
<tr>
<td>Western Interior</td>
<td>Hell Creek, Dogie Creek, Sussex, Lance Creek, Teapot Dome, Raton Basin</td>
<td>0.5-1</td>
<td>2250-2500</td>
</tr>
<tr>
<td>New Jersey</td>
<td>ODP 174AX</td>
<td>0.2-1</td>
<td>2500</td>
</tr>
<tr>
<td>Bermuda Rise</td>
<td>DSPD 396</td>
<td>0.5-1</td>
<td>2800</td>
</tr>
</tbody>
</table>

5.2.4 Accretionary Impact Lapilli

The basic mechanism we propose for the formation and growth of accretionary impact lapilli is similar to the formation and growth of accretionary particles created in pyroclastic flows (Figure 5.3 c). In pyroclastic flows lapilli form in one of two ways: either a large solid particle collects smaller solid particles that are coated in a thin layer of water or a large drop of water collects solid particles. Laboratory experiments show that both of these mechanisms are capable of making accretionary particles (Gilbert and Lane 1994). We propose a mechanism similar to the mechanisms put forward by Gilbert and Lane (1994) except the liquid agent in our model is molten rock, although any condensable material in the ejecta curtain could potentially act as the binding agent. This
molten rock could condense directly onto small solid fragments from the vapor phase or could come from collisions with melt droplets.

Following Gilbert and Lane (1994), the collisional volume swept out by an accreting particle per unit time is:

\[ V_c = \frac{\pi}{4} (d_l + d_f)^2 \Delta U \]  \hspace{1cm} (5.8)

where \( d_l \) is the diameter of the large accreting particle and \( d_f \) is the size of particles it accretes. Additionally, \( \Delta U \) is the relative velocity between the large and small particles. Motivated by observations of accretionary impact lapilli, we assume that \( d_l \gg d_f \), and therefore \( d_l + d_f \approx d_l \). The mass of a single accreting particle therefore increases at a rate

\[ \frac{dM}{dt} = V_c wE = \frac{\pi}{4} d_l^2 wE \Delta U \]  \hspace{1cm} (5.9)

where \( w \) is the mass loading of small particles in kg/m\(^3\) and \( E \) is a dimensionless factor that accounts for all of the variables that affect the collection efficiency. One important contribution to \( E \) is the tendency of small particles to follow streamlines more closely than larger particles, so that the small particles may be swept around the growing accretionary lapillus instead of colliding with it. Another factor is the probability that a small particle that collides with the growing lapillus will actually stick. There is also the possibility that electrostatic attraction or repulsion could change the efficiency factor. By treating \( E \) as a free parameter, we avoid much of the complexity of the process of accretionary impact lapilli formation. Later we will determine \( E \) empirically by fitting our results to a known impact.
Assuming that the lapillus is spherical, it has a mass

\[ M = \frac{\pi}{6} d_l^3 \rho_l \]  \hspace{1cm} (5.10)

where \( \rho_l \) is the average density of the accreting lapillus.

Differentiating equation 5.10 with respect to time, we find

\[ \frac{dM}{dt} = \frac{\pi}{2} d_l^2 \rho_l \left( \frac{dd_l}{dt} \right). \]  \hspace{1cm} (5.11)

Then combining equation 5.9 and equation 5.11 we find the growth rate

\[ \frac{dd_l}{dt} = \frac{wE\Delta U}{2\rho_l}. \]  \hspace{1cm} (5.12)

To estimate \( \Delta U \), we need to consider the turbulent flow in the ejecta curtain. The low viscosities of silicate melt or vapor and high ejection velocity of distal impact ejecta imply a high Reynolds number flow (Peter Goldreich Priv. Comm.), which is inevitably accompanied by turbulence. The Reynolds number is defined as \( Re = \rho vL/\eta \), \( \rho \) is the density of the fluid, \( v \) is the flow velocity, \( L \) is the length scale of the flow, and \( \eta \) is the viscosity of the fluid. The turbulent flow is described by the length scale \( l_{turb} \), which is the size of the largest eddies in the flow. In most cases \( l_{turb} \) is set by the geometry of the flow and in our case \( l_{turb} \) is expected to be comparable to the thickness of the melt layer in the ejecta curtain. The other parameter used to describe the turbulent flow is the velocity scale \( v_{turb} \), which is the velocity of the largest and fastest eddies. The velocity scale is some fraction of the flow velocity and can be written as \( v_{turb} = v_{flow} f \), where the fraction \( f \) is called the turbulent intensity. For our geometry the flow velocity is not equal to the ejection velocity but is instead the relative velocity of adjacent portions of
the ejecta curtain. The flow velocity can be approximated as
\[ v_{\text{flow}} \approx \frac{dv_{ej}}{dR} \cdot l, \]
where \( l = l_{\text{turb}} \) is the thickness of the melt sheet, \( v_{ej} \) is the ejection velocity of material and \( R \) is the radial distance from the point of impact to the material in question. For an overview of important aspects of turbulent flows see Tennekes and Lumley (1972).

We assume that the small particles have almost no inertia and move with the enclosing fluid. Additionally, we assume the accretionary particles are only loosely coupled to the fluid and hence move independent of turbulence on small length scales. Under these conditions, the growing accretionary impact lapilli will collide with small particles at the turbulent velocity (Abrahamson 1975). Thus,

\[ \Delta U \approx v_{\text{turb}} = f \cdot l_{\text{turb}} \cdot \frac{dv_{ej}}{dR} \]  

(5.13)

Where \( l \) is the turbulent length scale is equal to or proportional to the thickness of the melt sheet, which is proportional to the total thickness of the ejecta curtain. From high resolution impact models, we can obtain the mass of material at a given ejection velocity, and as shown in Figure 5.8,

\[ M(v_{ej}) \propto v_{ej}^{-4.8 \pm 0.1} \]  

(5.14)

for a 20 km/s impact velocity. The thickness of the ejecta curtain, \( l(v) \) at the time of ejection is expected to be proportional to this mass. Additionally, hydrodynamic scaling tells us that \( l \propto R_{\text{imp}} \) thus \( l \propto v_{ej}^{-4.8 \pm 0.1} R_{\text{imp}} \).

We must estimate the mass loading or mass per unit volume, \( w \), of the ejecta curtain before we can estimate the size of the accretionary impact lapilli. The density of the
ejecta curtain is not constant and so neither is the mass loading $w$. In Appendix B.3 we derive the following expression for average mass loading of the ejecta curtain from the time when lapilli start to form, $t_0$, to a later time $\tau$.

$$< w > \approx 1.2 \frac{p(t_0)}{\tau} \left( \frac{dv}{dr} \right)^{-1}$$

Assuming $E, \rho_l \approx \rho(t_0)$, and $v_{turb}$ are constant in time, the diameter of an accretionary particle is given by:

$$d = \frac{dd}{dt} \tau \approx 0.6 Ef l_{turb} \propto \nu_e^{-4.8 \pm 0.1} R_{imp}$$

At an ejection velocity of ~3 km/s, our hydrocode model gives $l_{turb} \approx 50$ m for a projectile diameter of 10 km. According to Tenekes and Lumley (1972), the turbulent intensity is on the order of $f = 0.01$ for a wide range of Reynolds numbers. Without any constraints on the collection efficiency and a poorly constrained turbulent intensity we are unable to make even order of magnitude estimates of the lapilli size. However, as equation 5.16 shows, we are able to estimate how accretionary impact lapilli size should depend on ejection velocity and impactor size. We can then constrain $f$ and $E$ by comparison with known ejecta sizes. Assuming $f = 0.01$, choosing $E \sim 0.005$ gives $d_i \approx 1.5$ mm comparable to the size of accretionary impact lapilli ejected at ~3 km/s by the Chixculub impact (Yancey & Guillemette 2008). This value of $E$ seems reasonable as during simple laboratory experiments of Gilbert and Lane (1994) $E$ took values from 0.01-1.

Using the above values for $l_{turb}, E,$ and $f$ we derive the following equation for accretionary impact lapilli size as a function of impactor size and ejection velocity.
Figure 5.12 shows that our estimated accretionary impact lapilli sizes agree reasonably well with the somewhat limited observations of accretionary impact lapilli in Chicxulub and Sudbury ejecta (Table 5.3). We believe this agreement acts help support our model for the formation of accretionary impact lapilli.

In addition to terrestrial data on ejecta size distribution we also have the dependence of ejecta particle size implied by the radar dark Venusian parabolas, which is given, in meters, by

\[ d_v = 2400 D^{-2.65\pm0.05} R_c^{1.03\pm0.33} \]  

(5.18)

where \( D \) is the distance from the point of impact where ejecta will be emplaced, in km, and \( R_c \) is the crater radius in km (Schaller and Melosh 1998). These radar dark parabolas are produced by interactions between ejecta particles and the zonal winds of Venus. As ejecta particles fall through the atmosphere they are transported downwind, the distance that the particles travel is a strong function of the particle size (Schaller and Melosh 1998, Vervack and Melosh 1992).

Using the crater scaling relations of Housen et al. (1983) we find that \( R_{imp} \propto R_c^{1.25\pm0.08} \) where \( R_c \) is the radius of the crater that the impact will create. The range in the exponent for \( R_c \) comes from allowing the scaling parameter \( \alpha \) to vary from its theoretical
minimum value $\alpha = 3/7$ to its theoretical maximum $\alpha = 3/4$. Then using $D \propto v_{ej}^2$ we find that
\[ d_l \propto D^{-2.4 \pm 0.05} R_c^{1.25 \pm 0.08}, \]  
(5.19)

Our derived lapilli size and the particle size implied by the Venusian parabolas have a similar dependence on $D$ and $R_c$. As Figure 5.12 shows, the sizes estimated for a Chicxulub sized impact are also in good agreement. This agreement implies that the Venusian parabolas are composed primarily of accretionary impact lapilli. Moreover, if the Venusian parabolas are composed of accretionary impact lapilli, this agreement strongly supports our model for accretionary impact lapilli formation. The predominance of lapilli in Venusian crater ejecta, compared to their relative rarity in terrestrial ejecta deposits, may be due to the high initial rock temperatures on Venus and the consequent higher likelihood of melting. The massive melt outflows associated with Venusian crater ejecta support this inference (Chadwick and Schaber 1993). The presence of additional melt and vapor could explain the why the Chicxulub ejecta particle sizes estimated using equation 5.18, based on observations of Venusian parabolas, are somewhat larger than the observed lapilli sizes (Figure 5.12). The extra melt and vapor could increase the efficiency factor, $E$, resulting in larger lapilli for the same impact conditions.
Figure 5.12 Accretionary Impact Lapilli Diameter as a Function of Ejection Velocity

The red diamonds represent the observed size of accretionary impact lapilli in Chicxulub ejecta taken from Table 5.3. The blue diamond represents the observed size of accretionary impact lapilli in Sudbury ejecta taken from Table 5.3. Ejection velocities are calculated using the distance from point of impact and assumes a typical 45 degree ejection angle. The comparison of model estimates and actual lapilli data assumes that a roughly 10 km diameter impactor striking with a velocity of 20 km/s formed the Chicxulub and Sudbury structures. The solid black line is an empirical fit to the data assuming \( d_l \propto R_{imp} v_e^{-4.8} \) (Equation 5.16) and an impactor diameter of \( \sim 10 \) km. The dashed gray line represents ejecta particle sizes estimated for a Chicxulub sized impact, \( R_c = 90 \) km. This estimate uses dependence of ejecta particle size on both crater size and ejection distance implied by the Venusian parabolas (Schaller and Melosh 1998, Equation 5.18).
Table 5.3 Observations of Average Sizes of Accretionary Impact Lapilli

Average size of accretionary impact lapilli found in Sudbury and Chixulub ejecta at several locations and distances from the point of impact.

<table>
<thead>
<tr>
<th>Impact Region</th>
<th>Location/Site</th>
<th>Reference</th>
<th>Average size of accretionary impact lapilli (cm)</th>
<th>Distance from impact site (km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chixulub Belize</td>
<td>Albion Island</td>
<td>1</td>
<td>1-2</td>
<td>300</td>
</tr>
<tr>
<td>Chixulub Texas</td>
<td>Brazos river</td>
<td>2</td>
<td>0.1-0.2</td>
<td>900</td>
</tr>
<tr>
<td>Chixulub New Jersey</td>
<td>Bass river</td>
<td>2</td>
<td>0.025*</td>
<td>2500</td>
</tr>
<tr>
<td>Sudbury Lake Superior</td>
<td>Michigan</td>
<td>3</td>
<td>0.5-1</td>
<td>500</td>
</tr>
</tbody>
</table>

1. Pope et al. (1999)
2. Yancey and Guillemette 2008
3. Pufahl et al. (2007)

* Size assumes lapillus in figure 8B is of typical size.

5.3 Discussion

As previously mention recent experimental work shows that the ANEOS EOS for silica tends to underpredict the entropy of material shocked to a given pressure (Kurosawa et al. 2012, Kraus et al. 2012). It is hard to say how a more accurate EOS would affect the dynamics of the Hydrocode simulation. However, the ANEOS EOS for silica does a good job at determining the shock pressure and particle velocity behind a given shock (Kraus et al. 2012, Melosh et al. 2007). Assuming that the peak shock pressures reached and timescale for release are unaffected by the EOS, for a given shock pressure material will reach the liquid vapor coexistence curve at a higher pressure (Kraus et al 2012). Because we assumed that fragmentation takes place at the critical pressure (Appendix B.2) this change would not affect the predicted droplet sizes. If the critical pressure were to increase as suggested by Kurosawa et al. (2012) this would result in slightly earlier
fragmentation times, higher strain rates, larger accelerations, smaller melt droplets, and melt fragments.

Our axisymmetric models restrict us to considering vertical impacts while the most probable impact angle is 45 degrees. It is however possible to make qualitative estimate of how ejecta product sizes will depend on position with respect to the impact direction. Because the ejecta curtain will be thicker in the down range directions (Shuvalov 2011) we expect that impact lapilli will be larger in the down range direction and smaller up range. Similarly we expect that material with a given ejection velocity will be ejected further from the point of impact in the down range direction. This will result in slightly smaller strain rates and accelerations at the time of fragmentation for this material. Ultimately, this will yield somewhat larger melt droplets and melt fragments in the down range direction and smaller ejecta product in the up range direction for material with the same ejection velocity.

Our simplified model has several limitations. Our size estimates for melt droplets and melt fragments depend on several parameters that are estimated to varying degrees of accuracy. Thus, our size estimates are only order of magnitude estimates. Although the current agreement between our size estimates and geologic observation is notable, the most important aspect of our estimates is the prediction of how melt droplet and melt fragment size depend on impactor size, impact velocity, and ejection velocity. The predicted decrease in melt droplet and melt fragment size with increasing ejection
velocity qualitatively agrees with geologic observations (Glass and Pizzuto 1994, Schaller and Melosh 1998).

Our size estimate for accretionary impact lapilli depends on the turbulent intensity and the collection efficiency, which are both poorly constrained. Thus, our model currently only predicts how the size of accretionary impact lapilli depends on impactor size and ejection velocity. This dependence agrees reasonably with the inferred sizes of impact ejecta particles that form the Venusian parabolas and observations of ejecta from Chicxulub and Sudbury. Assuming the Venusian parabolas are indeed composed of accretionary impact lapilli, this agreement supports our model of the formation of accretionary impact lapilli.

Although our model indicates some dispersion in melt droplet sizes, our simple model only estimates the average size of the ejecta products and does not attempt to estimate the size distributions of these products. Expansion of our model to include more detailed microphysical modeling would allow us to estimate the size distribution of the ejecta products. This type of modeling would also allow us to make rudimentary estimates of the relative abundances of the different ejecta products. Such a model would likely have to be coupled directly to a two-dimensional or three-dimensional impact hydrocode such as iSALE and could prove to be prohibitively computationally expensive.

It is important to note that our work has focused predominantly on comparisons with the Chicxulub ejecta. This focus is made out of necessity, as the K-Pg boundary layer is the
only layer with readily available data on ejecta product size as a function of distance from the source crater. Additionally, Chixculub represents one of the largest known craters on Earth and allows us to “safely” disregard atmospheric effects that will be more prevalent for smaller impacts. A more detailed comparison of our models to known ejecta layers will allow us to test the predicted dependence of ejecta product size on impactor size and may even allow us to empirically constrain some of unknown or weakly constrained parameters of our model.

The inclusion of more realistic microphysical modeling and a more realistic EOS in a three dimensional model should not change the major qualitative aspects of the model presented here. One important finding is that the largest melt fragments will come from more lightly shocked near surface target material that does not reach the point of incipient vaporization. This is consistent with geochemical and isotopic observation of tektites showing that tektites come from near surface target material. Another important finding is that melt droplets, melt fragments, and accretionary impact lapilli form early in the impact process, well before emplacement or re-entry into an atmosphere. Our model also predicts that these ejecta products should be found together in well preserved ejecta curtain layers and that all three products should form even on bodies without atmospheres or significant volatile content. The prediction that ejecta curtain layers should contain melt fragments, melt droplets, and accretionary impact lapilli, sometimes having significantly different sizes is in good agreement with observations of Chicxulub and Sudbury ejecta (Yancey and Guillemette 2008, Addison et al. 2005).
Our model brings several assumptions regarding the outer suevite at Ries into question. The highly irregular flattened shapes of some “melt bombs” found in the outer suevite are taken as evidence of formation in a vapor rich secondary plume created by interactions between the craters hot melt sheet and inflowing water (Stöffler et al. 2013). Although our work cannot necessarily account for the “knife sharp” contact between the Bunte Brecia and the outer suevite (Stöffler et al. 2013), the relative velocity of melt and vapor particles during normal ejecta transport can explain the shape of these melt particles. Additionally, Artemieva et al. (2013) argue that the presence of accretionary impact lapilli implies that abundant water was involved in the crater suevite formation. Here we have argued that the formation of accretionary impact lapilli does not require water. Although we have focused predominantly on terrestrial ejecta layer our model can also be applied to extraterrestrial impacts and may help researchers test the controversial hypothesis that the “Martian spherules” are accretionary impact lapilli (Knauth et al 2005).
Appendix: Detailed calculations

B.1  Hydrodynamic similarity and scaling

We can scale our results for a 10 km diameter impactor to any size impact using hydrodynamic similarity. If we neglect gravity, the equations of hydrodynamics are invariant under the following scale transformation,

\[ t' = \beta t, \quad (B.1) \]
\[ x' = \beta x, \quad (B.2) \]
\[ v' = v, \quad (B.3) \]
\[ a' = \frac{a}{\beta}, \quad \text{and} \quad (B.4) \]
\[ \rho' = \rho \quad (B.5) \]

where \( t \) is time, \( x \) is the position coordinate, \( v \) is the velocity, \( a \) is the acceleration, \( \rho \) is density, and \( \beta \) is a scaling parameter. If we change the size of the impactor from \( R_{imp} \) to \( \beta R_{imp} \), we can determine the scaling of the ejecta product sizes using the equation B1-B5. For example, melt droplets size \( d_m \propto a^{-\frac{1}{2}} \), this corresponds to \( d_m \propto R_{imp}^{\frac{1}{2}} \).

Although less robust than size scaling, we can assume simple velocity scaling such that

\[ a \propto \frac{v_{imp}^2}{R_{imp}} \text{ and } d_m \propto a^{-\frac{1}{2}} \propto V_{imp}^{-1} R_{imp}^{\frac{1}{2}}. \]
B.2 Tracer analysis

In an Eulerian hydrocode material moves through a fixed mesh or grid of cells. Unlike a Lagrangian hydrocode, the motion of an individual parcel of material is not tracked in an Eulerian code. For this reason we use Lagrangian tracers to track the motion and thermodynamic path of a parcel of material with time. Each tracer has a position that is known at sub-grid resolution. The velocity of the tracer is estimated by linearly interpolating the calculated nodal velocities, in the fixed Eulerian mesh, to estimate the velocity at the position of the tracer. The pressure and temperature of the tracer are estimated to be equal to the temperature and pressure calculated for the cell they are in. Because the pressure and temperature are assumed to be uniform throughout an Eulerian cell, a certain amount of numerical “noise” appears in this tracer data when a tracer moves from one cell to the next. Applying the appropriate smoothing filter eliminates this noise. We save the pressure and position of the tracers about once a millisecond. Using this data we can obtain the pressure (Figure B.1), position, velocity (Figure B.2) and acceleration (Figure B.3) of a tracer as a function of time. The velocity and acceleration are calculated from the position and time using a time centered difference. As shown in Figure B.1, we estimate that fragmentation occurs when the pressure drops below the critical pressure of $P_c = 1.89 \times 10^8$ Pa. Using this fragmentation time we can obtain the position of the tracer at this time for our melt fragment calculation. Using the fragmentation time we also estimate the maximum acceleration after fragmentation occurs as shown in (Figure B.3). The results of our analysis of 35 tracers are reported in Table B.1.
In reality the pressure at which fragmentation occurs depends on the peak shock pressure obtained by the material as this determines where material comes to the liquid vapor coexistence curve. Using the expected intercept pressures for the tracers proved to be problematic due to a certain amount of “smearing” of the Lagrangian parcels. We found about 1/3 of the tracers reached almost constant pressures, like those in Figure B.1 after 3.3 s, before the material should have reached the liquid-vapor coexistence curve. Once material reaches the liquid-vapor coexistence curve its temperature and pressure drops more slowly (Johnson and Melosh 2012a). Thus when a tracer’s pressure or temperature becomes roughly constant, it implies that the material has reached the liquid-vapor coexistence curve. To avoid this issue of tracer “smearing” we adopted the critical pressure as a proxy for when fragmentation occurs. Considering the uncertainties associated with our already admittedly unrealistic choice for the equation of state, e.g. using pure silica and the problem with under predicting the entropy of material shocked to a given pressure (Kraus et al. 2012, Kurosawa et al. 2012), assuming the fragmentation pressure is constant seems reasonable. This uncertainty in the estimated fragmentation time may be the largest source of error in our calculations of melt droplet and melt fragment sizes.
Figure B.1 Pressure as a Function of Time for One Tracer.

Pressure as a function of time for the tracer with initial position $x_0 = 4987.5$ m and $y_0 = -212.5$ m, for a 10 km diameter impactor and 20 km/s impact velocity. The horizontal gray line acts as a guide for the eye to show the critical pressure, $P_c = 1.89 \times 10^8$ Pa, an estimate of the pressure at which material will intersect the liquid-vapor coexistence curve. At $t_{frag} = 0.323$ s the pressure drops below the critical pressure and we assume that fragmentation has occurred.
Figure B.2 Velocity as a Function of Time for One Tracer.

Velocity as a function of time for the tracer with initial position $x_0 = 4987.5$ m and $y_0 = -212.5$ m, for a 10 km diameter impactor and 20 km/s impact velocity. The ejection velocity is estimated as the velocity at a time of 3 seconds when tracer and corresponding parcel of material are in ballistic flight, meaning only gravity is acting to accelerate the material. The black dashed line acts as a guide to the eye to show $t_{frag} = 0.323$ s.
Magnitude of acceleration as a function of time for the tracer with initial position $x_0 = 4987.5$ m and $y_0 = -212.5$ m, for a 10 km diameter impactor and 20 km/s impact velocity. The smoothed acceleration, which is used to estimate the maximum acceleration after fragmentation, is obtained by time averaging the x and y acceleration over ~10 ms (10 save steps) and then finding the total acceleration. This is done to remove some of the noise caused by tracers moving through cell boundaries. The dashed line acts as a guide to the eye to show the time of fragmentation $t_{frag} = 0.323$ s. The acceleration at the time of fragmentation is $a = 4342$ m/s$^2$. Shortly after fragmentation, ~0.4 s and on, the magnitude of acceleration is roughly constant at 200-300 m/s$^2$. Looking at Figure B2, it is obvious that there is little change in the velocity of the tracer during this time. This roughly constant magnitude of acceleration is the result of excess numerical noise that has not been removed by our smoothing. A similar ~100 m/s$^2$ acceleration is seen at early times before the shock wave has even reached the tracer.
Table B.1 Compiled Tracer Data.

Data compiled from 35 tracers for a 10 km diameter impactor and a 20 km/s impact velocity. \( x_0 \) and \( y_0 \) are the initial x and y positions of the tracers, \( v_{ej} \) is the ejection velocity, \( t_{frag} \) is the time of fragmentation, \( a \) is the maximum acceleration experienced by the tracer after fragmentation, and \( R_f \) is the x position of the tracer at the time of fragmentation.

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B.3 Mass loading of ejecta curtain

The density of a parcel of material with constant mass is given by

$$\rho(t) = \frac{M(t_0)}{Vol(t)} \quad (B.6)$$

and

$$Vol(t) = 2\pi R(t) \times l(t) \times \Delta R(t) \quad (B.7)$$

where the geometry of the system is described by figure B.4. Thus, if $t_0$ is the time of ejection

$$R(t) = R_{ej} \left(1 + \frac{V_{ej}}{R_{ej}} \cos(\theta)(t - t_0)\right) \quad (B.8)$$

$$l(t) \sim l(t_0) \quad (B.9)$$

and

$$\Delta R(t) = \Delta R(t_0) \left(1 + \frac{V_{ej}}{R_{ej}}(t - t_0)\right) \quad (B.10)$$

so that

$$\rho(t) \approx \frac{\rho(t_0)}{\left(1 + \frac{V_{ej}}{R_{ej}} \cos(\theta)(t - t_0)\right) \left(1 + \frac{V_{ej}}{R_{ej}}(t - t_0)\right)} \quad (B.11)$$

Now we must estimate the time-averaged mass loading from the time when accretion starts, $t_0$, to some later time $\tau$. Assuming that $t_0 \ll \tau$, we find

$$< w > = \frac{1}{\tau - t_0} \int_{t_0}^{\tau} \rho(t) dt \approx \frac{\rho(t_0)}{\tau} \left(\frac{dv}{dr}\right)^{-1} \left(\frac{\ln(\cos(\theta))}{\cos(\theta) - 1}\right) \quad (B.12)$$

and for a typical ejection angle of ~45 degrees, $< w > \approx 1.2 \frac{\rho(t_0)}{\tau} \left(\frac{dv}{dr}\right)^{-1}$. 
Note that if we add a time dependence for \( l(t) = l(t_0) \left(1 + \frac{v_{ej}}{R_{ej}} C(t - t_0)\right) \), where \( C \) is some constant, we still find that \(<w> \propto \frac{\rho(t_0)}{r} \left(\frac{dv}{dr}\right)^{-1} \).

Figure B.4 Geometry of Ejecta Curtain.

Schematic illustration describing the simplified geometry of the ejecta curtain. The schematic shows the ejecta curtain at two different time \( t_1 \) and a later time \( t_2 \). The dimensions and position of the same parcel of material, which has a mass \( M \), are denoted at both times.
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- NS Mackie Endowed Scholarship (2007)
- Class of 1965 Endowed Scholarship (2006)
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- Parkos, D., Alexeenko, A., Kulakhmetov, M., Johnson, B. C., Melosh, H. J. NOx from Impact Ejecta Reentry Caused the End-Cretaceous Marine Extinction. (draft for submission to *Nature*)
- Johnson, B. C. and Bowling, T. J. Spherule layers abound but where have all the craters gone? (submitted to *Geology*)
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**Invited Talks:**


**Contributed Talks:**


