MODELLING THE COLLISIONS OF INTERSTELLAR DUST GRAINS WITH MOLECULAR DYNAMICS SIMULATIONS

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ABSTRACT

Dust grains and the ices that form on their surfaces are persistent through many astronomical environments, from large molecular clouds to protoplanetary disks. Collisions between dust grains are a means for grain growth to occur, especially at lower velocities, which is a key step in planet formation. Grain-grain collisions are also a means for ices on the grain surfaces to be ejected into the gas phase, where they may be observed via rotational transitions. This investigation uses a molecular dynamics approach to simulate collisions between dust grains encased in amorphous water ice, with a focus on the threshold between sticking and non-sticking behaviors in the parameter space of collisional velocity and impact parameter. As well as collisions between identically sized dust-grains, differently sized grain pairings are also explored. The threshold for sticking versus non-sticking collisions is found to be higher in velocity for identical grains than for differently sized grains (with maximums of $10^{3.3}$ m/s versus $10^{3.25}$ m/s, respectively). In many collision scenarios, water molecules were found to ejected from the ice mantle and lost to the gas phase.

1 INTRODUCTION

Interstellar clouds are made up of gas particles, of both atomic and molecular species, and microscopic dust grains. The dust grains, which have populations composed of either carbonaceous or silicaceous material, make up approximately 1% of the total mass, and range approximately from nanometer to micrometer scales (Weingartner & Draine 2001). While many chemical reactions can occur in the gas phase of these molecular clouds, the gas-phase molecules and atoms can also adsorb onto the surface of the dust grains, facilitating chemical reactions. At the low temperatures of the grains, typically around 10 K, chemical reactions between surface species results in products that are retained on the grain surfaces, building up ice mantles which gradually cover the grain in its entirety. The most abundant species on the grain surfaces is water (H_2O); however, other simple species, including carbon monoxide and dioxide (CO, CO_2), ammonia (NH_3), and methane (CH_4), make up a significant proportion of the ice mantles. The precise composition of the ices varies, dependent upon the chemical makeup of the molecular clouds Potapov et al. (2020). Water and the other species which makeup the mantles of these grains can also act as the starting platforms for the formation of more complex molecules, which are an object of interest for several areas of astronomy Herbst (Herbst).

Collisions between dust grains has the possibility of leading to sticking between them, forming larger structures Ossenkopf (1993). Grain growth from these collisions continues until the dust structures are large enough to interact gravitationally, in the contexts of planet formation. In higher velocity collisions, in the opposite regime, collisions can result in the breaking up of mantle structures and decomposition of larger dust grains or dust-grain aggregates, knocking off compounds formed on the grains into the gas phase. The details of the velocity and angles at which these different results will happen is an object of interest, especially considering the extra variables of icy mantles, which have been found to be really common. Molecules such as water, with relatively strong intermolecular forces between the individual molecules as well as with the surfaces of these grains, have the ability to act to increase attraction between grains at short distances, while also deforming to absorb energy, which can increase the sticking efficiency.

2 METHODS

In this study, we have used a purpose-built molecular dynamics code to simulate collisions between spherical, interstellar, carbonaceous dust grains coated with water ice. Parameters such as grain core size, ice mantle thickness, impact parameter, and velocity, were varied in order to explore the effects that these changes had on the collision characteristics, focusing mainly on the relative velocities and impact parameters. The thresholds of velocity and impact parameter at which the collisions resulted in sticking or non-sticking outcomes were studied. Prior to the collision calculations, the same code was also used to create the dust grains and to deposit the ice mantles onto their surfaces. The details of molecular dynamics model as well as the methodology used to explore the grain collisions are explored further in this section.

2.1 Molecular Dynamics Code

Molecular dynamics, the simulation technique used in this investigation, is a well-studied and utilized method in a variety of

fields, especially chemistry. It entails simulating the trajectories of a system of particles in time by numerically integrating classical equations of motion that describe the aforementioned system. Ahead of conducting these simulations, a suitable and computationally feasible set of interaction potentials and behaviors must be chosen in order to provide the best representation of the system. This deterministic method of tracking particle motion gives an approximate means of simulating a system's behaviors with a known set of chosen interactions. The particular method of implementing this technique in the molecular dynamics code was the Velocity Verlet algorithm E. Carlon & Nomidis (2015). This scheme allows the positions to be calculated accurately up to the fourth order in time while only storing memory of position, velocity, and acceleration for one increment per time step, reducing memory storage and increasing efficiency.

The MD code used here was built from scratch with the explicit purpose of simulating icy grain collisions as well as creating the underlying grain and ice-mantle structures. A set of potentials was laid out in order to describe the interactions occurring between each of the simulated species, which in this first treatment concerns only the water molecules of the ice mantle and the carbon atoms of the amorphous carbon core. The specific potentials used were chosen to provide a realistic degree of accuracy to the behavior of the species (water, carbon), while also maintaining manageable simulation times. These potentials were implemented via a box-grid method, which assigns molecules to boxes in the position space considered by the code, so that the potentials are considered for molecules only in boxes nearby to one another. Actual cutoffs in the potentials define the range of the forces involved, as described below. The code treats the water molecules atomistically, adopting intramolecular potentials that allow internal energy to be considered; this is essential to ensure that all degrees of freedom are fully considered, especially during the higher-energy grain-grain collisions.

2.2 Model Potentials and Grain Structure

The MD collision simulation first required the creation of both the dust grains as well as their icy mantles. The grain core was chosen to be made of amorphous carbon, considered to be one of the common components of interstellar dust grains. Silicate grain cores, another common component of astronomical dust grains, were not used in this study, but differences in their behaviors may be explored in future investigations of this model.

The chemical interactions between carbon atoms of the same grain were enacted using a set of potentials developed by Tersoff (1988). These empirical, interatomic potentials for carbon were originally developed for treating silicon, but adapted in terms of the parameter values to describe carbon. This relatively simple but realistic approach gives an accurate description of the structure and energy calculations for carbon, which motivated its use in this model.

In most of the simulations presented here, carbon atoms in different dust grains do not interact with each other, as they are surrounded by water ice. However, in some cases, the grain surfaces themselves may indeed come into contact. Carbon atoms of different grains were assumed in this model not to interact chemically, thus requiring an alternative to the Tersoff potential for these interactions. We use the van der Waals potentials for sp^3 carbon provided by Cornell et al. (1995); these were designed to be fully compatible with the TIP-3P potential that we use here for the water-water interactions.

Depending on the coordination of the carbon atoms within the grains, the Tersoff potentials can approximate sp, sp^2 or sp^3 bonding. Thus, at the outer surfaces of the grains, some carbon atoms would be potentially reactive. While we avoid this possible problem by allowing the Tersoff potentials to act only between carbon atoms originating in the same grain, in the interstellar medium it is to be expected that any reactive carbon atoms on the surface of the grain would soon chemically react with H atoms from the gas phase, removing any immediate reactivity.

However, at high collision speeds, the assumption of the grains being chemically inactive with each other might break down. With sufficient energy, the structure of the grains could be disrupted, breaking chemical bonds and allowing reactions directly between carbon atoms in either grain. Here, we adopt a moderate enough range of speeds in these collision simulations that, combined with the ice mantle covering of the grains, makes the use of this assumption reasonable. A specific investigation of high-speed collisions between bare grains, for example, would likely require the introduction of hydrogenated carbon in the construction of the dust grains.

The potentials and structure chosen for this model were motivated by several factors. Water was chosen as the sole mantle constituent as water is believed to be the main component of interstellar ice mantles of dust grains. Water also has a larger temperature at which it is goes from the solid phase on the grain to the gas phase, meaning it likely plays a larger role in the dust grain collisions where the temperature is warmer. Protoplanetary disks, for example, in the outer regions of the disk where the dust and gas is cooler, is likely to be an area where these collisions are important. The specific model of water behavior and associated potentials was chosen as the TIP3P model. TIP3P is an isotropic, three-site potential model for water, in which partial charges are placed on the oxygen and hydrogen atoms, with a 6–12 potential acting between oxygen atoms. It is an older but well-studied model of water behavior that produces a reasonably accurate treatment of water behavior while maintaining simplicity and computational efficiency that was desired for the beginning treatment of this astrophysical problem. In tandem with the TIP-3P potential, intramolecular potentials are adopted following Dang & Pettitt (1987), which are fully compatible with TIP-3P.

The water molecules were additionally allowed to interact with the carbon atoms in the grains via a set of 6–12 potentials developed by Cornell et al. (1995), which are again compatible with TIP3P water potential.

2.3 Creation of Grain and Mantle

Prior to the simulation of the collisions, the two independent grains had to be created and initialized for their use in the model. The grain structure, previously described, is composed of an amorphous carbon core surrounded by a water ice mantle. The bare dust grains were produced by placing carbon atoms in an overall spherical shape, with their relative positions determined by a cubic lattice structure. The newly created grain was then annealed at high temperature, 2000 K in the framework, using a Berensen thermostat. The grain was then thermostated down to 500 K, then again to 100 K.

After the creation and relaxation of the carbon core struc-

ture, a water ice mantle was deposited onto the dust grain. Water molecules were added in layers around the carbon core structure consistent with the thickness desired for the model. The water molecules were initially placed in a simple cubic structure around the surface of the carbon grain. To ensure the production of an amorphous water structure (the expected structure of interstellar water ice), the orientation of the water molecules was randomized across the surface of the carbon grain. The combined water and carbon structure was then thermostated at 100 K to relax the structure.

A process of back-filling of any gaps or pores within the water structure was then carried out, followed by another period of relaxation at fixed temperature of 100 K.

The above process ensures that non-porous ice mantles are considered in these simulations. While the porosity of water-ices deposited onto grains has been shown to be significant Raut et al. (2007) in the laboratory, other experimental studies, as well chemical kinetic models, have shown that ices that are formed chemically on grain surfaces instead of being directly deposited are likely much more compact Oba et al. (2009). Thus, while our method of building the water ice involves a kind of direct deposition, it was deemed to be more realistic to use a compact ice with no gaps/pores in the present models. It is likely that porosity in the ices would change the collisions dynamics and thus the model outcomes. We leave the investigation of such effects to future studies.

The back-filled and relaxed water-ice/dust grain combination was then thermostated from 100 K down to 10 K, creating the final structures of icy-dust grains utilized in the collision simulations. The finalized cross-section of the grains used in each of the collision scenarios are shown in Figure **??**.

A similar process was undertaken for making larger and smaller grains than shown in the previous figure. The thickness of water ice in these grains was kept the same, while the sizes of the carbon core was changed, allowing exploration of collisions between identical and differently sized grains. Each of the icy grains made prior to the collision simulations were thermostated to 10 K, which is a typical characteristic temperature of assumed for dust grains in dark interstellar clouds. The temperatures of other astronomical environments in which icy dust grains are likely and may undergo collisions can be higher in some sources, or may vary within an individual sources, such as protoplanetary disks. Such variations were not explicitly considered in this study. A characterization of the size of the core, mantle, and mass/number of particles for each of the main dust grains explored in the model is shown in Table 1.

2.4 Icy Dust Grain-Grain Collisions

Following creation of the icy dust grains using the MD code and other processes, the simulation of the collisions between grains were explored. The variety of models ran focused on the effects that the fractional impact parameter and relative velocity of the collisions had on the outcomes, specifically sticking or non-sticking. The two grains' centers of mass were set a specified distance away from each other, outside any interaction potential cutoff significant in the model. The relative velocity, one of the two main parameters changed in the model space, was assigned inversely by the mass, i.e. a grain with 10 percent of the total mass of the two grains would be assigned a velocity that was 90

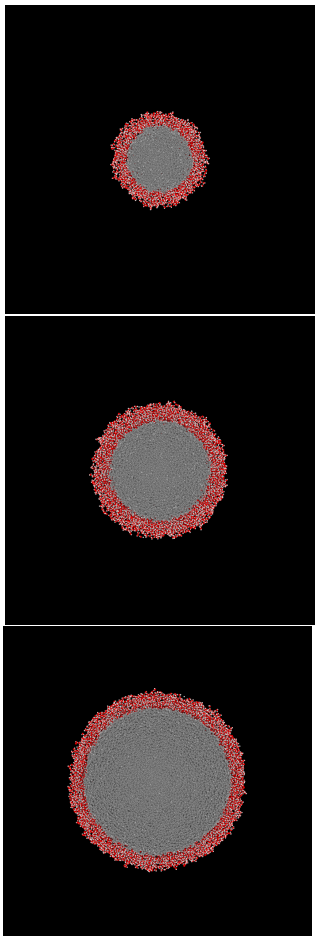

Figure 1. These images display the cross section of the small, medium, and large grains from top to bottom. The red indicates water molecules and the gray indicates the carbon of the grain. All of the grains have the same thickness of water layer, but differing size of the carbonaceous grain.

percent of the relative velocity for that model. In the collisions involving the equal mass grains, each grain is assigned a velocity half of the relative velocity. The starting positions of the grains were altered to fit the fractional impact parameter of the specific model. The fractional impact parameter for a grain collision as the distance between the centers of mass of the two grains where they narrowly don't overlap over the distance between the actual centers of mass of the grains in the collision. Fractional impact parameter, b, is shown below:

$$b = \frac{R_{CM}}{R_0} \tag{1}$$

Where R_{CM} is the distance perpendicular from the collision path between the centers of mass in the model, and R_0 is the sum of the radii of the two dust grain + ice mantles. A fractional impact parameter of 0.9 represents a grazing collision between the two colliding grains, where a fractional impact parameter of 0.0 represents a head-on collision. The fractional impact parameter was used a parameter instead of the more common impact parameter as it is more easily scalable to changing grain sizes.

For identically-sized dust grain collisions, several ranges of velocities were investigated, primarily to find the thresholds between sticking and non-sticking for the icy dust grains. The velocities

Table 1. Table Characterizing The Size of the Different Grains Used

Grain Label	Number of Water Molecules	Number of Carbon atoms	Total Number of Molecules/Atoms
Small	5434	11017	16451
Medium	14388	37501	51889
Large	23607	121861	145468

chosen were logarithmic in nature, initially starting with 100, 1,000, and 10,000 m/s for relative velocities. The fractional impact parameters were considered in 0.1 increments from 0 (head-on collision) to 0.9 (glancing collision) for each relative velocity, meaning 10 model runs for velocity increment investigated. Following the initial velocity values chosen, relative velocities were chosen in order to narrow the gap between velocity values of primarily sticking collision results and primarily non-sticking collision results. The parameters chosen for the model runs of identically-sized dust grains are fully detailed in the results, along with images displaying their end states. In order conserve computer resources and time, not all models were run for the same overall amount of time. The priority for each model was determining the end result of the collision between the colliding dust grains. The models were stopped after POV-Ray imaging showed clear separation of the colliding objects or the overall structure of the two now joined grains no longer displayed overall changes. For instance, collisions with 10 Km/s relative velocity interact and collide at much shorter timescales than that of 100 or 1000 m/s collisions, allowing a shorter overall simulation time to provide needed information.

For different-sized dust grains, similar ranges of velocities were explored to investigate differences in the impact-parameter space for changing dust grain sizes. The thickness of the ice layers are the same between all sizes of simulated dust grain, with the carbon core size being the main factor changed. The velocities and impact parameters at which the various simulations took place at can be seen in Figure 8.

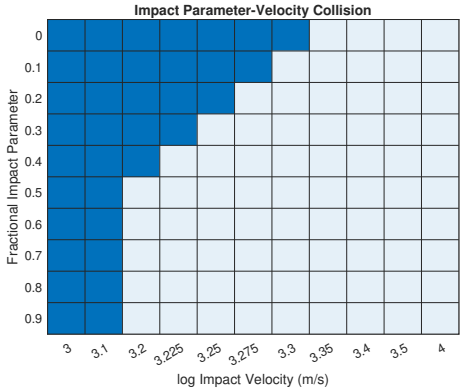

Figure 2. This figure represents the results of identically-size grain simulations, where blue tiles are simulations that resulted in the grains sticking , and the light grey are simulations where the grains did not stick together. The x-axis represents the log(base-ten) of the impact velocity of the two grains.

3 RESULTS & DISCUSSION

The total number of simulations for the combination of the identical icy grain collisions and the large-small icy grain collisions summed over 100 models, which could take anywhere from one week for fast, conclusive collisions, to several weeks. The main focus lent on the outcome of these collisions in order to gain more information about at what velocity grain collisions stick.

3.1 Collision Results

Models were continued until understanding in the velocity-impact parameter space of the identical-size and large-small collisions was obtained. Patterns in the velocity-impact parameter space visibly differed in two collision situations observed. A map of the tested parameter space for both the situations can be found in Figures 2 and 8.

3.1.1 Identically-Sized Collisions

The initial investigation into this MD model of grain collision involved the collision of identically-sized molecules. The medium grain structure, shown in Figure 2.3, were used. The parameter space was explored by determining whether the grains stuck or not at largely varying velocities, and running models interspersed in the velocity space to see finer detail in the threshold of where the grains stuck or not. The results of the identically-sized collisions are shown in Figure 2.

The highest velocity at which the two grains stuck to each other was that at $10^{3.3}$ m/s, with an impact parameter of 0.0, indicating a head-on collision. The highest velocity at which the two grains stuck at impact parameters 0.1-0.9 also shown in 2. The identically-sized collisions had many sticking collisions when the velocity lowered, with the sticking collisions at 0.9 at 10^{3} m/s. Although the darker color indicates a sticking-collision, not all of the collisions that were classified into these two categories were identical in their appearances. Gentler, lower velocity collisions could collide where no molecules were knocked off of either grain, and the ice mantle did not deform much, like in Figure 3.

Additionally, in collisions closer to the sticking threshold that still resulted in sticking collisions, more water molecules were lost from the grain system and the final shape of resulting grain/s is more deformed. The differing in the shapes of the two is likely to have an impact in the further collisions with the combined new grain. An example of a sticking collision that's final structure is more stretched is shown in Figure 4.

Classification of the collisions as non-sticking also had a variety of qualitative outcomes within the category. The non-sticking collisions that barely separate, especially at lower impact parameters, showed deformed structure similar to the sticking collisions on and had a more gradual separation after the initial impact. This type can be shown in Figure 5. Other collisions, which had high impact parameters (glancing collisions), tended to also eject

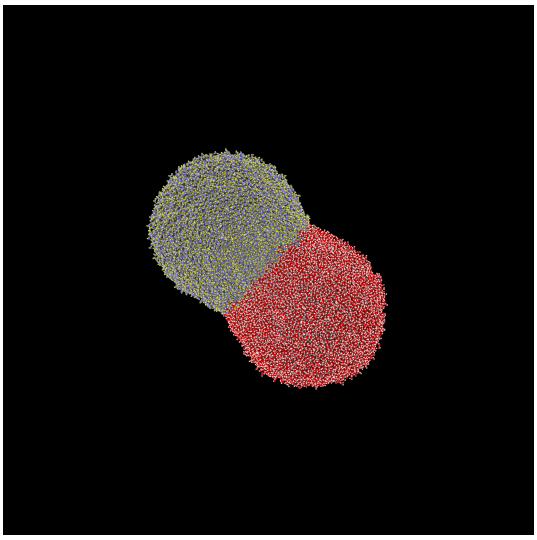

Figure 3. Gentler, sticking collision, with a fractional impact parameter of 0.0 and a velocity $10^{3.1}$ m/s

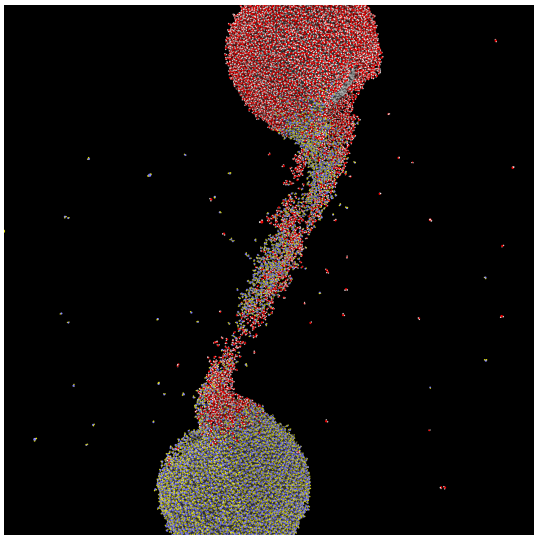

Figure 5. Non-Sticking collision between identically-sized grains, with a fractional impact parameter of 0.4 and $10^{3.275}$ m/s. This type of slower separation ejects less molecules.

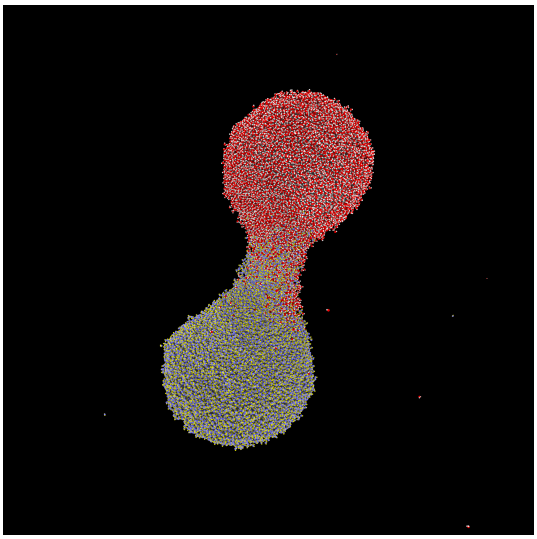

Figure 4. Sticking collision between identically sized grains, with a fractional impact parameter of 0.2 and $10^{3.25}$ m/s

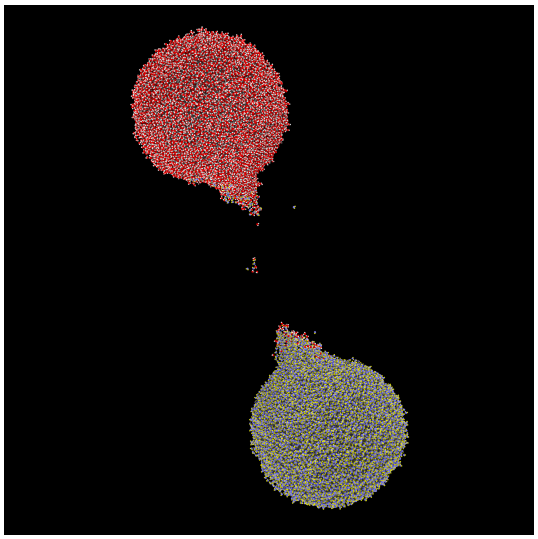

Figure 6. Non-Sticking collision between identically-sized grains, with a fractional impact parameter of 0.9 and $10^{3.225}$ m/s. This high impact parameter collisions only involves low cross-section, and much smaller amounts of water molecules are ejected.

small amounts of material, even at higher speeds, mostly due to the small collision cross-section between them 6.

More violent collisions tend to lie further from the threshold, as expected, where large numbers of water molecules are ejected from these grains.These more violent collisions, which may result from astronomical events such as shocks and protostellar outflows, could be an important mechanism for the loss of grain material. An example of these collisions from the identical grain model space is show in Figure 7

3.1.2 Large-Small Collisions

After getting finer resolution in the velocity-impact parameter parameter space, the attention was shifted to collisions between grains of different size. One method of obtaining relative velocity between dust grains for collisions is turbulence and vorticity, which deferentially affects grains of different sizes Harju et al. (2020). The grid of the results of the collisions between the large-small grains are shown in Figure 8, where dark blue indicates a sticking collision and the light blue indicates non-sticking collision. The largest velocity at which the grains stuck at was $10^{3.25}$ m/s, unlike the higher barrier of of $10^{3.3}$ for the identically size grains. The large-small grains were also less likely to stick together at higher impact parameters and slower velocities compared to the identically sized-grains.

Like the identical types of collisions, there were similar categories of collisions among the broader categories of sticking vs. non-sticking collisions. Under sticking collisions, those closer to the threshold formed more deformed and extended structures, like

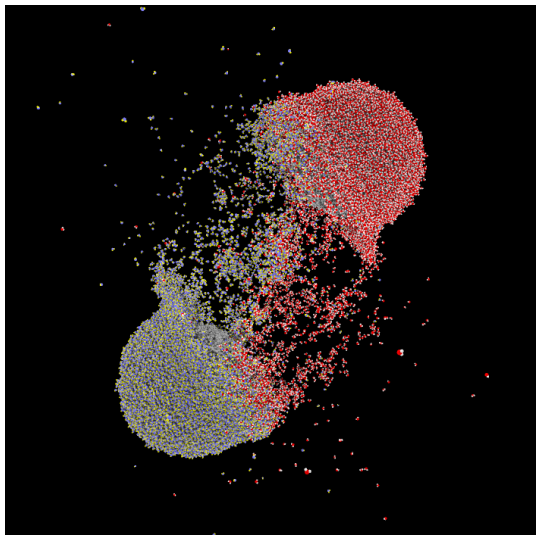

Figure 7. Non-Sticking collision between identically-sized grains, with a fractional impact parameter of 0.4 and $10^{3.275}$ m/s. This type of slower separation ejects less molecules.

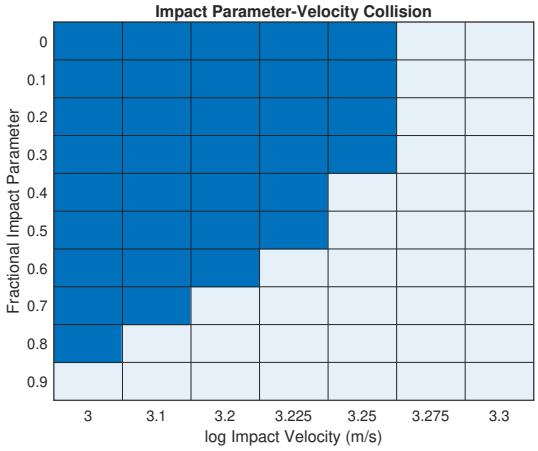

Figure 8. This figure represents the results of simulations between the icy grain collisions of differing size, where blue tiles are simulations that resulted in the grains sticking , and the light grey are simulations where the grains did not stick together. The x-axis represents the log(base-ten) of the impact velocity of the two grains.

in Figure 9. In slower and smaller impact parameter collisions, very few or no molecules tend to be ejected, an the structure is more uniform, shown in Figure 10.

In the non-sticking collisions, more direct collisions at faster velocities that are close to the sticking/non-sticking threshold formed large trails of molecules along the axis of collision, although eventually leading to a non-sticking result. These types of collisions eject molecules from the grain system much slower and are subject to forming larger cluster left behind from these trails, shown in 11. With sufficient velocity, the result becomes large removal of water molecules from the grains, seen in Figure 12. As seen in the heat maps of the identical and large-small grain collisions, the non-sticking occurs at a lower velocity for the large-small collisions.

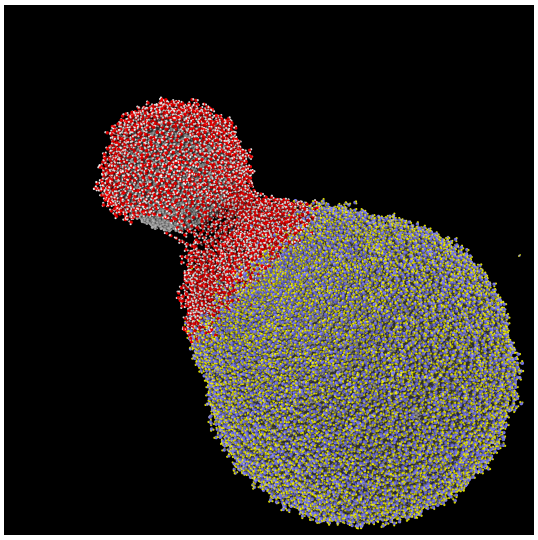

Figure 9. Sticking collision between different-sized grains, with a fractional impact parameter of 0.0 and $10^{3.25}$ m/s. This collision tends to eject more molecules although the final result was sticking between the grains. The structure of the resulting combination is noticeably different from gentle collisions.

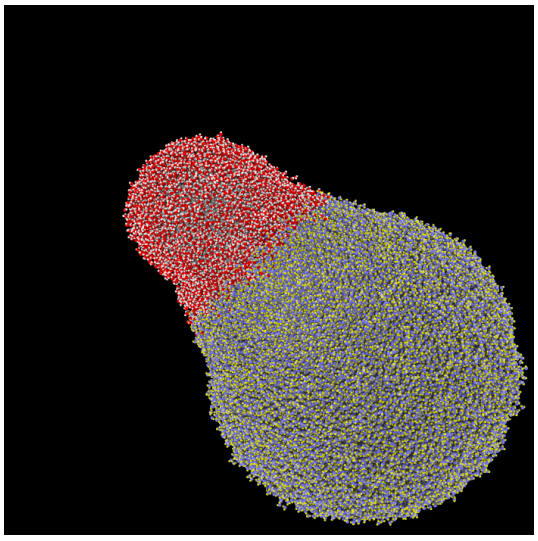

Figure 10. Sticking collision between different-sized grains, with a fractional impact parameter of 0.0 and $10^{3.2}$ m/s.

3.1.3 Comparison between Varying Size Icy Grain Collisions

The large-small dust grain collisions tended to stick at lower velocities compared to identically-sized grains. Common between all of the types of icy dust grains used in the models is the thickness of the icy mantle. The ratio of the icy mantle thickness and mass of the large grain material to the water mantle is lower for the larger grains than for the smaller grains. Some additional simulations were conducted with increasingly small mantle thicknesses on the colliding grains, which may represent more realistic conditions, especially in planet forming conditions where temperatures are warmer and the grains themselves are canonically larger than simulated in these experiments. The current MD model for the

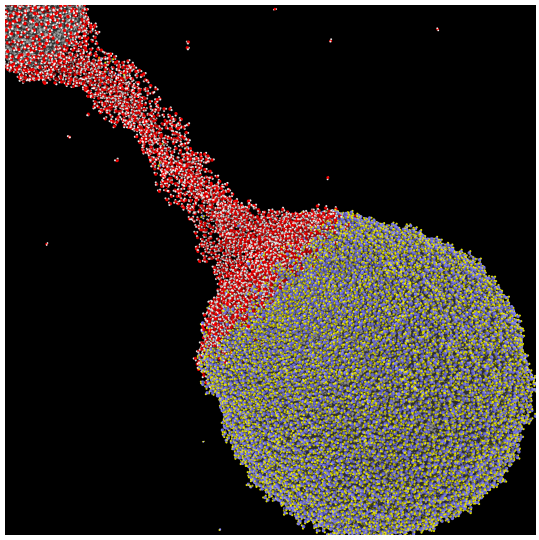

Figure 11. Non-sticking collision between different grains, with a fractional impact parameter of 0.0 and $10^{3.275}$ m/s. The smaller grain eventually becomes disconnected from the system.

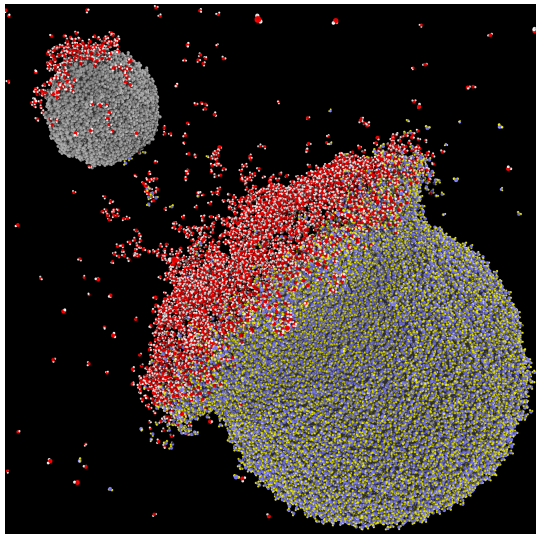

Figure 12. Non-sticking collision between different grains, with a fractional impact parameter of 0.0 and $10^{3.4}$ m/s.

grain collisions, when applied to slower collisions with more interaction between the bare carbon grains, showed lower colliding velocities. However, these situations may require more careful potentials between interacting species to be employed, especially with respect to the carbon-carbon potentials of opposite grains.

There were distinct differences between the sticking vs. non-sticking thresholds seen for the large-small grain collisions and the identical-size grain collisions. The primary parameters of these types of collisions tested were velocity and impact parameter. There are likely several other parameters that may determine whether a collision sticks or not. One important consideration is the size of the grains being simulating. In MD and in this model in particular, the potentials, forces, velocities, and positions are calculated for each particle and all of the interactions within range of each other. The computational power required to conduct these simulations limits the amount of particles and the size of the grains that can be simulated. The grains used in these simulations are on the order of nanometers in size, with the water mantle as a sizeable portion of this radius. While the sizes of the mantles in actual astronomical environments is likely to vary based on how long molecules have had to accumulate, the thickness of the mantle compared to the grain size is likely very large in these simulations compared to astronomical environments. This may be one explanation for the large velocity of sticking observed in these experiments. Lower mantle thickness and lower velocity collisions may require a more careful treatment of the potentials over short distances, and could produce lower velocity sticking threshold. More investigation into the average mantle thickness on these dust grains would further inform these simulations.

4 CONCLUSIONS

Through the molecular dynamics simulations of astronomical icy dust grain collisions, a more explicit view of the threshold between sticking and non-sticking in these collisions has been investigated, for collisions involving identically-size dust grains as well as differentially-sized dust grains. Fast, energetic collisions, of which are characteristic for astronomical events such as shocks and protostellar outflows, were shown to be able to eject a lot of the water material making up the mantle of these grains. However, even collisions that stick were shown to cause water molecule to reach the gas phase, indicating that grain collisions may be an important mechanism for some molecules formed on dust grains to leave the grain at cold temperatures.

Comparing the collisions that involve identical grains and those that involved collisions between a large and small dust grain, the identical dust grains were seen to stick at higher velocities for the same angle of collision or impact parameter than the large and small grain collisions. The maximum velocity at which grains stuck in these simulations for the identical grains was $10^{3.3}$ m/s, compared to $10^{3.25}$ m/s of the collisions between large and small collisions. The high velocity nature of these thresholds may suggest that lower water mantle thicknesses should be employed in future studies of these types of collisions, especially as literature values for ice thicknesses improve. This type of future study could require more careful and computationally intensive potentials for water-water, water-carbon, and carbon-carbon.

Future work could also include the use of different common molecules on the surface of interstellar dust grains, such as CO/CO_2 or NH_3, or mixes of these species with water, to see how sticking depends on the difference in the composition of the ice mantle. Work on quantifying the number of water molecules lost, transferred, and lost in clusters, is currently being conducted, which will provide more quantitative summaries of how well these collisions eject water into the gas phase or into solid-phase clusters.

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