THE STOCHASTIC, IMPACT-INDUCED CRYSTALLIZATION OF PRIMORDIAL AMORPHOUS WATER ICE. J.K. Steckloff*[1], G. Sarid[2], B.C. Johnson[3], *Correspondence: jsteckloff@psi.edu, [1]Planetary Science Institute (Tucson, AZ), [2]SETI Institute (Mountain View, CA), [3]Purdue University (West Lafayette, IN).

Introduction: Amorphous water ice (AWI) is a solid, glassy phase of water ice that forms in the conditions of the solar nebular and proto-planetary disk [1,2]. AWI later incorporated into icy silicate grains and accreted together to form the original population of cometary bodies in the outer solar system [3], and may survive to the present day. Nevertheless, AWI has never been conclusively detected on an icy body's surface in the present Solar System [4].

Pure amorphous water ice can spontaneously and irreversibly transition into crystalline water ice, releasing a significant amount of energy on the order of ~10^5 J/kg [5]. Because of these energetics, the crystallization of AWI is often thought to be the energy source driving cometary outbursts, explosions and dust jet activity [6-13]. Additionally, AWI's ability to release trapped gases upon crystallization has been thought to explain the production of common highly-volatile species [14,15]. However, AWI-free mechanisms have been proposed to explain all of these cometary behaviors [16-21]. Additionally, impurities reduce the exothermicity of AWI's crystallization, and can render the crystallization *endothermic* if concentrations of common volatiles reach a few mole percent [22].

Furthermore, collisional evolution may crystallize AWI. In particular, Nice-style instabilities in the early Solar System [23-25] are thought to have led to significant collisional evolution of the primordial comet population [26], potentially leading to significant shock-induced crystallization of any primordial AWI in icy bodies. This begs the question: could amorphous water ice even survive this early collisional environment?

Methods: To compute the amount of AWI that crystallizes during an collision between icy bodies, we use iSALE to simulate these impacts, and then feed these outputs into an AWI crystallization script.

Planet migration and iSALE simulations. The proto-Edgeworth_Kuiper Belt objects were likely ~100km-sized objects [27] that collided with one another at typical impact speeds of ~2-4 km/s [26]. To study such impacts, we use iSALE, an arbitrary Lagrangian-Eulerian impact shock-physics code [28]. Although there is no sufficient amorphous water ice equation of state (EOS) for iSALE, a water ice EOS can reasonably approximate AWI due to their similar densities. We use the Eka-ANEOS equation of state for water [29], which describes the thermodynamic conditions of interest with sufficient accuracy. We assume that the initial AWI contains ~2-3% impurities of other volatiles, such that its crystallization is no longer exothermic [22]. We ignore all phases of water ice other than AWI and ice I, and use the same strength model as [30]. Furthermore, we assume that these objects have zero porosity for simplicity. We use iSALE's lagrangian tracer particles ("tracers") to record the temperature and pressures over time of the parcel of ice in which each tracer is embedded. We use a resolution of 250 grid-cells per object radius, which balances numerical accuracy while keeping runtimes to a few weeks, and record tracer data every 0.25 seconds.

AWI crystallization. The chemical potential controls phase transitions, with molecules spontaneously moving into phases that minimize their chemical potential. A temperature-dependent fraction of the amorphous water ice molecules will have enough kinetic energy to break their bonds and diffuse into a crystalline structure. Because the chemical potential of crystalline ice is always lower than that of AWI, ice will remain crystalline once crystalized [31]. [32] used these considerations to derive the temperature-dependent crystallization rate of AWI, and benchmarked their equations against experimental data. We use a modified form of this model to compute the fraction of remaining AWI that crystallizes in a single time step.

We feed the thermal history of each iSALE tracer through this model to compute the amount of AWI that crystallizes throughout the process, which is specific to each tracer. We then also aggregate these tracer AWI crystallization fractions, to determine how much of the initial AWI crystallizes and the degree to which this AWI crystallizes. In practice, we find that little of the initial AWI only partially crystallizes, as nearly all of the initial AWI is either fully crystallized (near 100%) or remains essentially uncrystallized (near 0%).

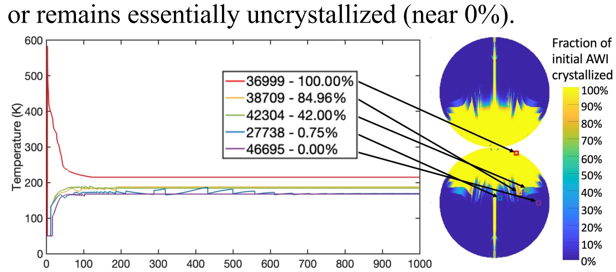

Figure 1: We plot the thermal profiles for five tracers in our simulation of two 100 km bodies at 50K colliding at 3 km/s. (*Left*) tracers in different parts of the body experience very different thermal profiles. Minor numerical artifacts are visible from a tracer passing between grid cells. (*Right*) We trace the tracers to their original locations in the bodies.

Results: We find that the amount of AWI that crystallizes is highly sensitive to impact speed. We consider relative impact speeds from 500 m/s to 5 km/s, and find that AWI crystallization is highly sensitive to impact speed across this range. At the slow end of this range (1 km/s and slower), negligible AWI crystallizes regardless of initial temperature. At the other extreme, no AWI survives uncrystallized, and nearly all AWI (~90%) fully crystallizes at 5 km/s. Extrapolating, it is clear that impacts slower than 500 m/s will also preserve essentially all AWI, while impacts faster than 5 km/s will cause nearly all AWI to fully crystallize.

Crucially, our results show that there is a wide range of outcomes between 2 km/s and 4 km/s, which is the expected variation in impact speeds during the early catastrophic collisional evolution of the proto-EKB following Nice-style instabilities [26]. This suggests that the resulting fragments and reaccreted bodies, which are thought to comprise the modern day population of comets, centaurs, and TNOs, likely exhibit significant stochastic variation in the preservation of any amorphous water ice present, with the amount of surviving primordial AWI depending sensitively on each object's collisional history.

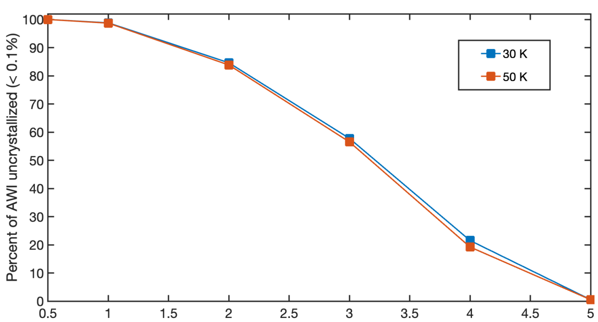

Figure 2: Fraction of initial AWI that remains uncrystallized as a function of impact speed for different initial temperatures. The crystallization dynamics of AWI is highly sensitive to impact speed; the amount of AWI that remains uncrystallized is particularly sensitive to the range of expected impact speeds between icy bodies during planet migration of 2-4 km/s [26].

Prior to the Giant Planet instability, the mean collisional velocities between proto-EKB objects varied from 780 m/s interior to 20 AU, down to 240 m/s beyond 25 AU [26]; these impact speeds are too slow to trigger significant AWI crystallization, suggesting that any primordial AWI would likely survive to the Giant Planet instability. At the time of the Giant Planet instability and onset of planet migration, collisional speeds are likely to be higher in the inner parts of the disk relative to the outer parts, likely producing a heliocentric gradient in the survival of AWI; with the amount of AWI surviving any average collision increasing with heliocentric distance. Finally, collision velocities are generally too low within the present Oort Cloud [33], TNO [34], and Centaur [34] populations to trigger significant AWI crystallization. Thus, any AWI that survives this early collisional processing is likely to experience no further significant impact-driven AWI crystallization over the age of the Solar System.

Conclusions: We find that impacts in the comet reservoir populations are much too slow to crystallize significant amounts of AWI. However, the impacts triggered by planet migration in the early solar system (~2-4 km/s) can strongly impact the amount of AWI that survives. Whereas at lower speeds (2 km/s) ~85% of AWI survives uncrystallized, this drops to only ~20% at 4 km/s. This suggests that the survival of AWI is highly sensitive to collisional history, with high-speed and/or highly collisional environments allowing little to no primordial AWI to survive to the present day.

References: [1] Mastrapa, R. M. E. et al (2013) In Gudipati, M. S. and Castillo-Rogez, J. eds., *Ap. & Spa. Sci. Lib.,* 356, 371. [2] Ciesla, F.J. (2014) *ApJL* 784:L1 [3] Weidenschilling, S. J. (2004) U. AZ Press, 97 [4] Lisse, C. et al. (2013) In Gudipati, M. S. and Castillo-Rogez, J. eds., *Ap. & Spa. Sci. Lib.,* 356, 455 [5] Ghormley, J. A. (1968) *J. Chem. Phys.* 48, 503. [6] Prialnik, D. and Bar-Nun, A. (1992) *A&A*, 258, L9 [7] Sarid, G. et al. (2005) *PASP,* 117, 796 [8] Prialnik, D. et al. (2008) *MNRAS*, 388, L20. [9] Sekanina, Z. (2009) *Int'l Com. Q.*, 31, 99 [10] Jewitt, D. (2009) *AJ,* 137, 4296 [11] Kossacki, K.J. and Szutowicz, S. (2013) *Icarus*, 225, 111. [12] Mousis, O. et al. (2015) *ApJ*, 814, L5. [13] Agarwal, J. et al. (2017) *MNRAS* 469, S606 [14] Bar-Nun, A. et al. (1985) *Icarus*, 63, 317 [15] Bar-Nun, A. et al. (2007) *Icarus*, 190, 655 [16] Crifo, J.-F. et al. (2002) *EMP*, 90, 227 [17] Kossacki, K.J. and Szutowicz, S. (2011) *Icarus*, 212, 847 [18] Combi, M.R. et al. (2012) *AJ*, 749, 29 [19] Grün, E. et al. (2016) *MNRAS*, 462, S220 [20] Steckloff, J. and Melosh, H.J. (2016) *AAS-DPS 54* Abstract #206.06 [21] Steckloff, J. K. et al. (2016) *Icarus*, 272, 60 [22] Kouchi, A. and Sirono, S.-i. (2001) *GRL*, 28, 827 [23] Tsiganis, K. et al. (2005) *Nature* 435, 459 [24] Morbidelli, A. et al. (2005) *Nature* 435, 462 [25] Levison, H.F. et al. (2011) *AJ* 142, 152 [26] Morbidelli, A. and Rickman, H. (2015) *A&A* 583, A43 [27] Morbidelli, A. et al. (2009) *Icarus,* 204, 558 [28] Melosh, H. J. et al. (1992) *JGR*, 97, 14735. [29] Turtle, E.P. and Pierazzo E. (2001) *Science* 294, 1326 [30] Bray, V. J. et al. (2014) *Icarus* 231, 394 [31] Speedy, R. J. et al. (1996) *J. Chem. Phys.*, 105, 240 [32] Kouchi, A. et al. (1994) *A&A*, 290, 1009 [33] Stern, S.A. (1988) *Icarus,* 73, 499 [34] Durda, D.D. and Stern, S.A. (2000) *Icarus,* 145, 220

Acknowledgements: This research is supported by NASA grant 80NSSC18K0497.