THERMODYNAMICS OF GIANT IMPACTS: RESULTS USING IMPROVED EQUATIONS OF STATE.

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Introduction. During terrestrial planet formation, the energy deposited by giant impact events leads to dramatic changes to the thermal and physical structure of the planet. As a result, giant impacts are major drivers of the chemical evolution of planets. Previous work has focused primarily on the effects of giant impacts on core formation because the elevated temperatures in a magma ocean are a strong influence on the partitioning of elements between metal and silicates. However, the chemical perturbations from giant impacts remain poorly characterized, largely due to the limitations in our understanding of the thermodynamics of planetary materials under the extreme conditions of giant impacts.

Over the last decade, the available data on the equations of state (EOS) of planetary materials have increased substantially due to both computational and experimental investigations over a wide range of pressures and temperatures (P-T). However, these data had not been utilized to improve the material models used in hydrocode simulations of giant impacts. Here, I present new EOS models for iron and an iron-alloy and the initial results from simulations of giant impacts between terrestrial planets using new EOS models for the mantles and cores.

Improved material models. It is challenging to construct an EOS model that spans the P-T range encountered in giant impacts [1]. The ANEOS code package [2] is able to produce a thermodynamically self-consistent multi-phase material model over nearly all P-T, but the complexity of the underlying physics is limited to relatively simple, classical formulations. Recently, Stewart et al. [3] updated the ANEOS code to include an additional input parameter that adjusts the heat capacity of the liquid. In the original ANEOS code, the thermal free energy term assumed a Dulong-Petit limit, but planetary liquids exceed this value. The new input parameter must be fitted to shock temperature or shock entropy constraints for each material. Stewart et al. [3] revised the EOS model for forsterite (Mg_2SiO_4) using the updated ANEOS code. The ANEOS source code [4] and forsterite parameters and documentation [5] are publicly available.

I constructed new EOS models for pure iron and an iron-silicon alloy ($Fe_{85}Si_{15}$) using the updated ANEOS code (in preparation for public release). The models include a single solid phase (γ-Fe), liquid and vapor. The updated model Hugoniots, based at STP, are in good agreement with available constraints on the shock temperatures and entropies [e.g., 6]; however, the ANEOS formulations are insufficient to accurately represent planetary materials over the entire P-T range of interest. The new iron-alloy and forsterite models produce a much better fit to Earth's present-day internal structure compared to previous EOS models used in hydrocode calculations. Note that the published literature contains multiple versions of 'ANEOS models' for iron and forsterite that use different input parameters and different features in the ANEOS code. The new EOS models for forsterite, a proxy for the mantle composition, and iron-alloy, a proxy for the core, provide much improved calculations for material temperatures compared to previous EOS models.

Giant impact calculations. These calculations used the GADGET2 smoothed particle hydrodynamics (SPH) code modified for planetary collisions (available with 7) with the new EOS models. I present an initial set of giant impacts that explores a range of impact energies, final planet masses, and initial thermal structure. The results were examined for sensitivity to resolution (number of particles) and for conservation of energy and angular momentum (AM). The nominal initial thermal structures were a fully solid mantle along the isentrope that intersected the forsterite melting point at the surface and a fully liquid iron-alloy core with an isentrope that intersected the peridotite solidus.

In collisions, energy is conserved within 1%, with the error primarily arising from imperfect exchange between potential, kinetic, and internal energies at the time of closest approach of the cores of the two bodies [8]. AM conservation is more variable and sensitive to the specifics of the impact event and the resolution. The canonical Moon-forming giant impact [9] produces some of the largest variations in AM and bound mass because (i) the outer disk and escaping material are primarily composed of condensed clumps that are very sensitive to resolution and (ii) the escaping material holds a substantial fraction of the total angular momentum budget. These results indicate that this example event is a poor benchmark case for comparisons between different codes. More vaporizing giant impacts have more consistent outcomes, which should be more suitable for discerning differences between numerical methods.

Code limitations. Giant impacts deposit energy heterogeneously in the colliding bodies [8], leading to strong thermal stratification. After gravitational equilibration, both the mantles and cores have strong entropy gradients. Interpretation of the details of the calculated temperatures is fraught with danger. Hydrocode calculations typically neglect important processes such as heat transfer by mixing/turbulence and material miscibility. Radiative cooling is limited for the main body during the timescales of giant impacts. However, we need temperature to understand the chemical effects from giant impacts, so we must examine the results with these limitations in mind.

Supercritical mantles. Partially-vaporized mantle is generated at the point of impact, and the initial silicate vapor atmosphere quickly encircles the bodies. The hot outer layers are further heated via secondary shocks generated by the large differential rotations in the outer layers of the body during gravitational equilibration. As a result, the vaporized outer layers of the planet begin buoyant and remain buoyant throughout the event and are unlikely to mix completely with colder layers below. In most cases, the outer region is pure vapor and the internal P-T profile transitions from vapor to supercritical fluid to liquid without intersecting the vapor curve. This result was found in the lowest energy cases considered, including graze-and-merge and hit-and-run collisions between two 0.13 $M_\oplus$ bodies. The lower mantle ranges from partially solid to a few thousand degrees above the forsterite liquidus, depending on the event. The ubiquity of supercritical profiles was also seen in calculations using the older forsterite EOS in GADGET2 [8,10]. The supercritical structure of a rocky planet after a giant impact appears to be a robust result.

Extremely hot metal. Interpretation of the temperatures of iron-alloy in the system is much more complicated. In all giant impact calculations, some of the metal core is heated to extremely high temperatures. In calculations of the canonical Moon-forming event using previously available iron EOS model in GADGET2, core material reached almost 70,000 K, a value that justly raises questions about the accuracy of the material model in the giant impact regime. Using the new iron-alloy EOS, the temperatures in the iron core reach about 20,000 K after gravitational equilibration. These temperatures are still questionable. A portion of the high-temperature core is generated by shocks from the differential rotation between the core and mantle and a portion is generated by shocked and compressed projectile core falling through the target mantle. Some core material is so hot that it remains neutrally buoyant in the mantle, with the amount of core material mixed into the silicates varying widely depending on the impact parameters. In general, the metal is much hotter than the adjacent mantle. Extremely hot metal will exchange heat and chemically react with the mantle; however, the numerical methods cannot capture these effects.

In all cases, some of the metal exceeds the P-T conditions required for miscibility of the MgO-Fe system [11]; in some cases, all of the metal exceeds this miscibility boundary. Although the natural system has a more complicated and variable composition, this comparison illustrates the likelihood that some metal and silicate will dissolve into each other during each giant impact during the growth of terrestrial planets. And as a result, the calculations cannot capture the true temperatures of the natural system without taking these processes into account.

In general, these new results lend support to the idea that metal and silicate will partially dissolve during giant impacts. Because the temperature structure is strongly heterogeneous, dissolution would be spatially variable. In the hot, low-pressure vapor, metal and silicate may form one continuous solution as found in [12]. In the P-T of the middle mantle, the two phases may be largely immiscible. And at the core-mantle-boundary, dissolution may be possible, forming a heavy liquid layer at the base of the mantle. As the system cools, some metal would exsolve from the liquid and fall to the core. Overall, even though giant impacts are extremely energetic and may drive some large-scale mechanical mixing, the magma ocean formed by the event is unlikely to have a homogenous composition because of the strong thermal gradients. The chemical and redox heterogeneity (e.g., FeO content) evolves as the mantle cools.

Moon formation. Recently, Hosono et al. [13] proposed that a canonical giant impact onto a proto-Earth with a magma ocean has a larger fraction of target material in the disk compared to a solid proto-Earth. Using the new forsterite EOS, the target body was initialized with a mantle that was fully solid, mushy (following the melt curve), and fully liquid in the upper mantle. All cases produced the same projectile mass fraction in the disk. The first contact of the graze-and-merge event transforms the proto-Earth into a supercritical body, so there is little difference in the outcome of the second contact that provides the torque to emplace most of the material into the disk.

Conclusions. New EOS models for silicates and metals significantly improve the accuracy of the calculated temperatures in giant impact events. However, substantial challenges remain in the interpretation of the numerical results because of neglected physical processes in most hydrocodes. These new EOS provide a deeper understanding of the thermodynamics of giant impacts and the ability to investigate new aspects of the chemical processes that occurred during planet formation.

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