IMPROVEMENTS TO ANEOS FOR MULTIPLE PHASE TRANSITIONS

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ANEOS

Accurate equations of state are of vital importance in impact calculations. Robust predictions of impact melt and vapour volumes require sophisticated equation of state representation, including accurately determined phase boundaries and two-phase regions.

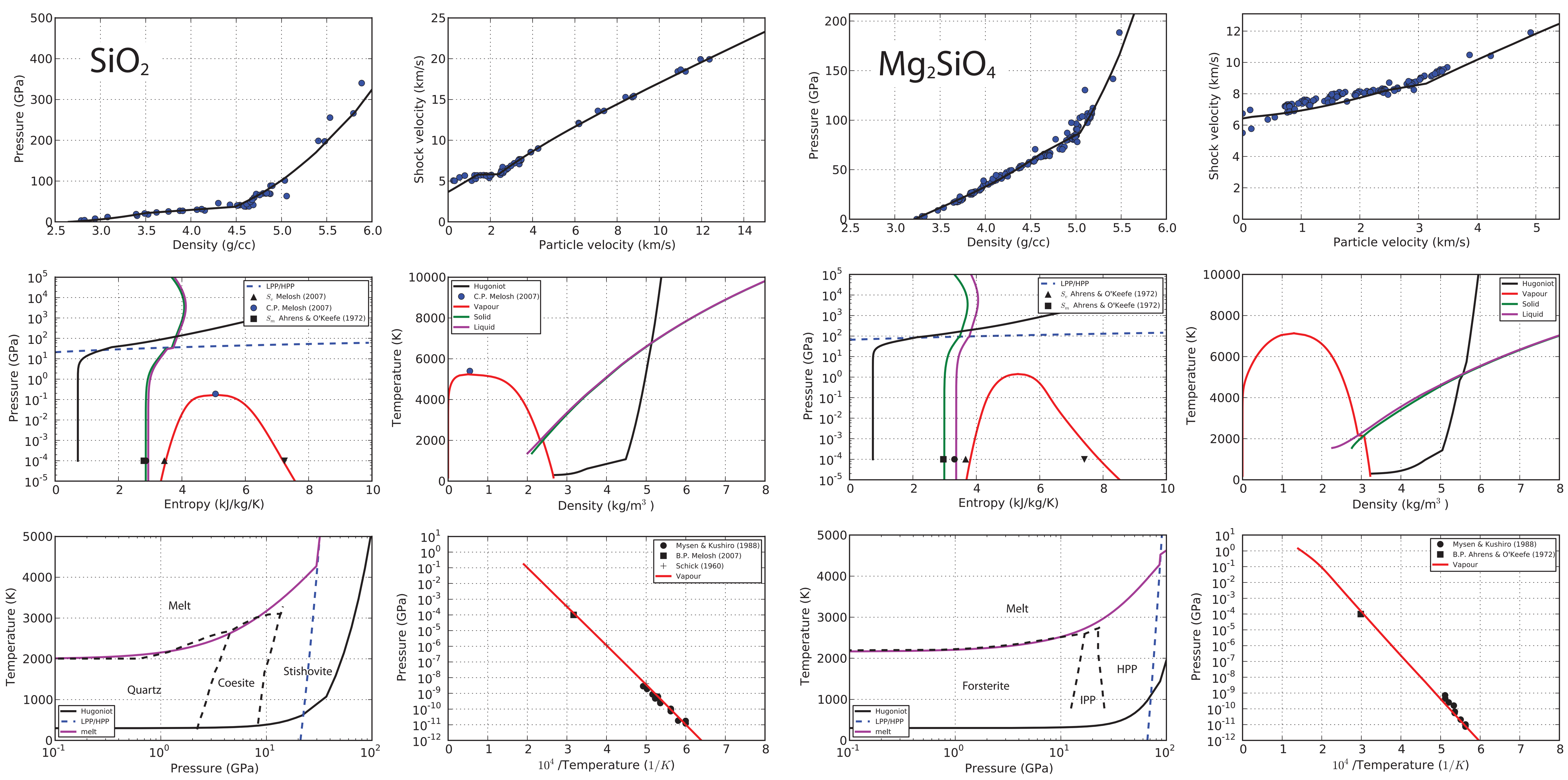
ANEOS is a complex computer program for calculating thermodynamically consistent equations of state, developed at Sandia National Laboratories [1, 2] and recently modified and improved for geological materials [3].

Although ANEOS is the most accurate equation of state package that is widely used in impact modelling, it is not without limitations. An important weakness in the treatment of the compressed region is that only one high-pressure solid phase transition can be included and it is accounted for by modifying the cold compression term alone [3, 4]. This implies that the experimentally observed dependence of phase transition pressure on temperature cannot be reproduced [3] and that the thermal expansion coefficient of the high pressure phase is the same as the low pressure phase [5], which can make it difficult to define realistic initial conditions in planetary impact simulations.

The fixed-pressure phase transformation also makes it difficult to locate the liquid/solid phase boundary. As a result, in the current version of ANEOS, liquid and solid states cannot be distinguished when a high-pressure phase transformation is included, and temperatures above the melt temperature are overestimated as latent heat of melting is not subtracted from the internal energy [3, 4].

Here we describe modifications to the ANEOS code to overcome these limitations and incorporate the improvements into the iSALE impact hydrocode package.

Melting in conjunction with existing method for treating solid-solid phase transition



In a first step, we added new routines to (a) locate and store in a table the liquid/solid phase boundaries in combination with the existing method for defining a solid/solid phase transition; and (b) given a specified density and temperature, use the liquid/solid transition table to identify the phase and calculate the mixed phase state if necessary.

This in-memory table method, which mirrors the approach used by ANEOS to locate the vapour transition, allows a (slower) more robust search algorithm to be used to locate the melt phase boundaries during the initial construction of the table, without reducing the efficiency of subsequent calls to ANEOS.

Linear interpolation is used to locate the phase boundary between points in the table and the lever-arm rule is used to compute the thermodynamic state in the mixed phase region.

When used in conjunction with a solid-solid phase transition, the tabulated melt curve is modified in the double mixed phase region by assuming a linear density-temperature relationship along the liquid and solid curves across the mixed-phase low- and high-pressure-solid region.

This approach has been successfully employed in the construction of equation of state tables for quartz (SiO_2, left) and forsterite (Mg_2SiO_4, right).

An improved treatment of solid-solid phase transitions

In a second, on-going step, following the success of recent multiphase equation of state development [e.g., 9] we are modifying ANEOS so that it treats high-pressure phase(s) as separate materials, with different thermodynamic constants.

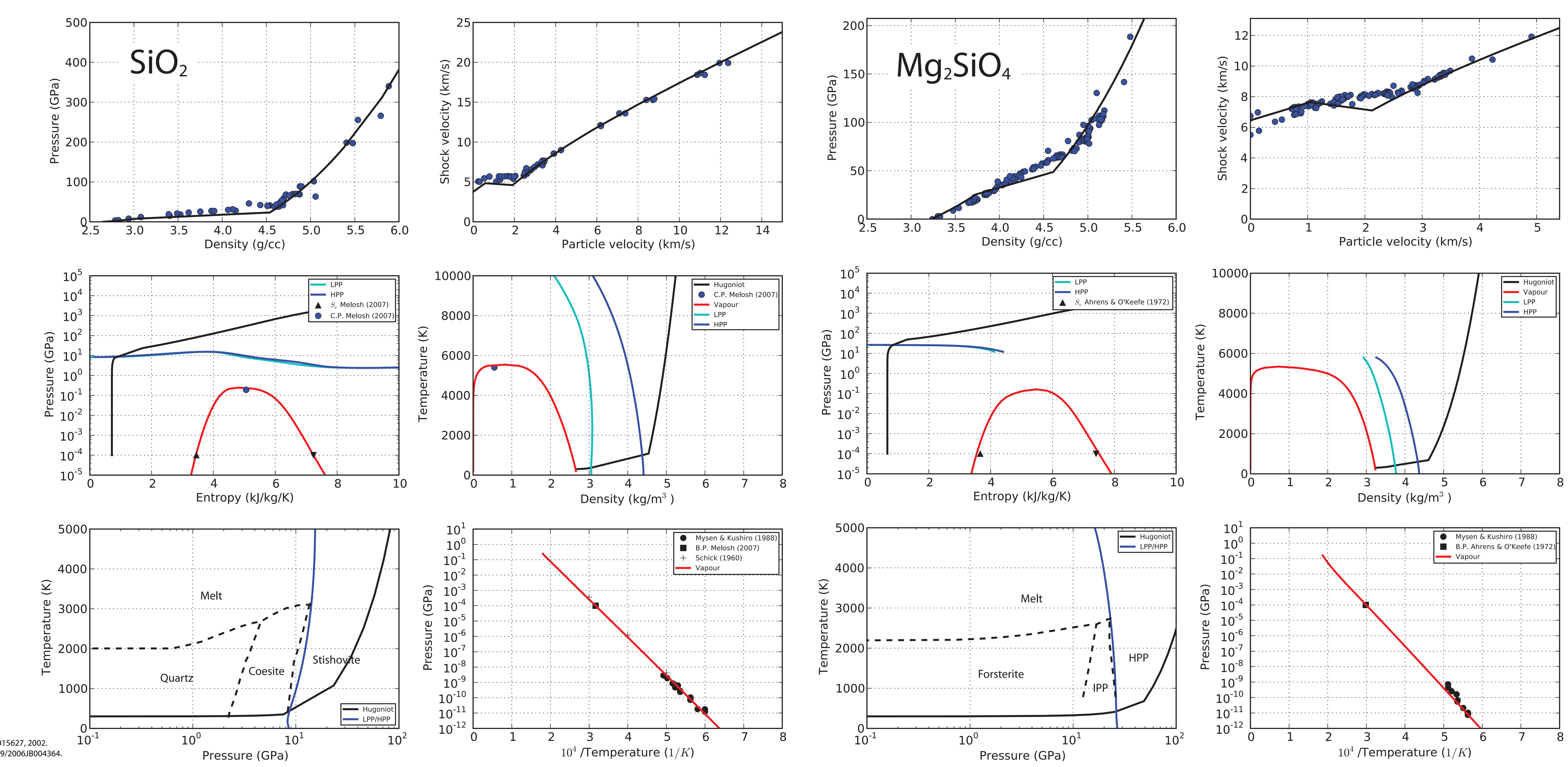
Phase boundaries are determined using a thermodynamic equilibrium approach analogous to that currently used to define the solid/liquid phase transition.

As with our modified melt transition method, the solid-solid phase transition information is stored in a table for subsequent use by ANEOS. Linear interpolation is used to locate the phase boundary between points in the table and the lever-arm rule is used to compute the thermodynamic state in the mixed phase region.

Preliminary results for quartz (SiO_2; left) and forsterite (Mg_2SiO_4; right) including one high-pressure solid phase and neglecting melting are shown. A remaining step is to combine this new solid-solid phase transition treatment with the new treatment of the melt transition.

ANEOS Parameter	Quartz (SiO_2) LPP[a]	HPP[b]	Forsterite (Mg_2SiO_4) LPP[c]	HPP
Density (g/cc)[d]	2.65	4.287	3.227	3.943
Bulk Sound Speed (km/s)	3.768	8.366	6.435[f]	7.4[d,f]
Gruneisen Gamma	0.618	*1.23*	*1.15*	*1.25*
Debye temperature (K)	650	1130	*736*	*853*
Slope of U-u_p	2.12	1.23[e]	1.06[f]	1.3[f]
Enthalpy of fusion (MJ/kg)[g]	0.156	N/A	0.81	N/A
Enthalpy of LPP/HPP transition (MJ/kg)	N/A	*1*	N/A	*1.2*

a) Melosh (2007) Meteoritics & Planetary Science 42(12), 2079–2098.
b) Wang, F. et al. (2012) J. Geophys. Res., 117, B06209, doi:10.1029/2011JB009100
c) Anderson, O.L. & Isaak, D. G. (1995) AGU Reference Shelf, 2, 64-97.
d) Smyth, J.R. & McCormick, T.C. (1995) AGU Reference Shelf, 2, 1-17.
e) Luo, S.-N., et al. (2002) Geophys. Res. Lett., 29(14), doi:10.1029/2002GL015627, 2002.
f) Mosenfelder, J. L., et al. (2007) J. Geophys. Res., 112, B06208, doi:10.1029/2006JB004364.
g) Navrotsky, A. (1995) AGU Reference Shelf, 2, 18-28.

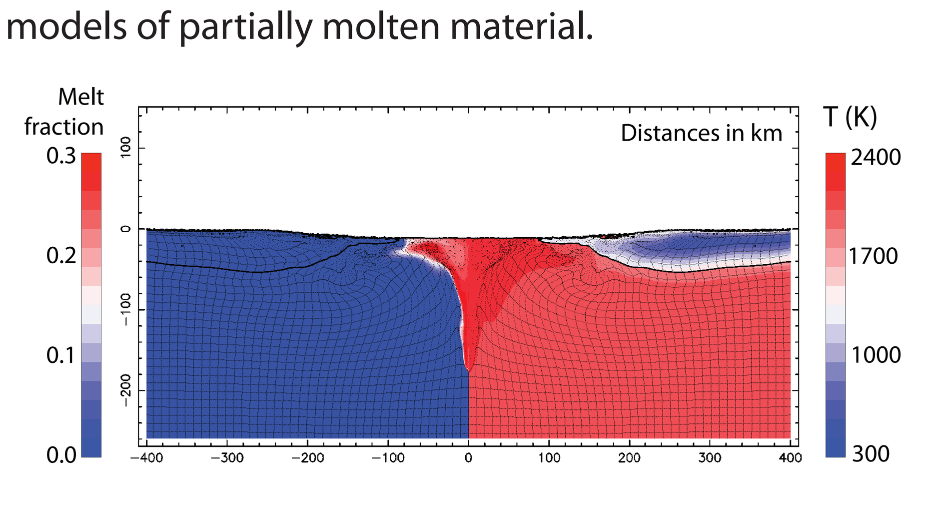


Discussion

To exploit the improvements made to ANEOS in this work, we have modified the iSALE hydrocode [10] to generate in-memory equation of state tables using ANEOS during problem start-up and to include entropy in the tables from which phase information can be deduced.

The omission of the melt transition in ANEOS-derived equation of state tables has been an important limitation of many previous impact modeling studies [e.g., 11]. Using new ANEOS parameters for forsterite that include both a solid-solid phase transition (old method) and a melt transition (with a high melt temperature of 2163 K, appropriate for pure forsterite), together with the epsilon-alpha porous compaction model, we found that post-shock temperatures above the melt transition can be over-estimated by as much as 660 K, which corresponds to a difference in shock pressure of 5-25 GPa, depending on initial porosity.

Inclusion of the melt transition also allows melt fraction to be estimated directly during an impact simulation from the specific entropy (below). In addition to improving the accuracy of melt-volume calculations, this will allow melt fraction to be used as a variable in rheological models of partially molten material.



Melt fraction (computed from entropy; left) and final temperature (right) distribution beneath a simulated lunar impact basin (52-km impactor diameter; 15-km/s impact velocity; 40-km crustal thickness; 35-K/km thermal gradient) using the SiO_2 (crust) and Mg_2SiO_4 (mantle; impactor) ANEOS equations of state with melting.

Conclusions

The improvements to ANEOS described here address long-standing limitations of the software that will aid the construction of accurate equation of state tables and improve future planetary impact simulations.

However, recent experiments have highlighted a further limitation of ANEOS [12, 13], which fails to correctly predict the entropy on the Hugoniot with the consequence that the shock pressure of vaporization is overestimated.

Future efforts will focus on addressing this shortcoming, as well as exploring mixture-model approaches for developing more realistic whole-rock equations of state by combining single-mineral equations of state, such as those developed for SiO_2 and Mg_2SiO_4.

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