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A New Wide-Range Equation of State for Xenon

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We describe the development of a new wide-range equation of state (EOS) for xenon. Three different prior EOS models predicted significant variations in behavior along the high pressure Hugoniot from an initial liquid state at 163.5 K and 2.97 g/cm^3, which is near the triple point. Experimental measurements on Sandia's Z machine as well as density functional theory based molecular dynamics calculations both invalidate the prior EOS models in the pressure range from 200 to 840 GPa [1]. The reason behind these EOS model disagreements is found to lie in the contribution from the thermal electronic models. A new EOS [2], based upon the standard separation of the Helmholtz free energy into ionic and electronic components, is constructed by combining the successful parts of prior models with a semi-empirical electronic model. Both the fluid and fcc solid phases are combined in a wide-range, multi-phase table. The new EOS is tabulated on a fine temperature and density grid, to preserve phase boundary information, and is available as table number 5191 in the LANL SESAME database [3]. Improvements over prior EOS models are found not only along the Hugoniot, but also along the melting curve and in the region of the liquid-vapor critical point.

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[1] S. Root et. al., Physical Review Letters 105, 085501 (2010).
[2] J. H. Carpenter et. al., EPJ Web of Conferences 10, 00018 (2010).
[3] http://t1web.lanl.gov/