

Abstract Submitted
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Silicon Nitride Equation of State¹ PAZHAYANNUR SWAMINATHAN, ROBERT BROWN², JHU/APL — This report presents the development a global, multi-phase equation of state (EOS) for the ceramic silicon nitride (Si_3N_4). Structural forms include amorphous silicon nitride normally used as a thin film and three crystalline polymorphs. Crystalline phases include hexagonal α - Si_3N_4 , hexagonal β - Si_3N_4 , and the cubic spinel γ - Si_3N_4 . Decomposition at about 1900 °C results in a liquid silicon phase and gas phase products such as molecular nitrogen, atomic nitrogen, and atomic silicon. The silicon nitride EOS was developed using EOSPro which is a new and extended version of the PANDA II code. Both codes are valuable tools and have been used successfully for a variety of material classes. Both PANDA II and EOSPro can generate a tabular EOS that can be used in conjunction with hydrocodes. The paper describes the development efforts for the component solid phases and presents results obtained using the EOSPro phase transition model to investigate the solid-solid phase transitions in relation to the available shock data. Furthermore, the EOSPro mixture model is used to develop a model for the decomposition products and then combined with the single component solid models to study the global phase diagram.

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²Robert C. Brown, my colleague of over 8 years, suddenly passed away Dec 9, 2013. This is largely based on his work and is presented as a tribute to him.

Pazhayannur Swaminathan
JHU/APL

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