

	Abstract Submitted	
	for the March 20-24 1995	
Suggested sessions	Meeting of the	March '95 Sorting
1. Materials Physics	American Physical Society	Category
2. Chemical Physics		15p (5f, 3a,g)

Non equilibrium carbon and its Effect on High pressure Equations of State of Mixtures. M. VAN THIEL and F. H. REE. Lawrence Livermore National Laboratory—The Statistical Mechanics of mixtures of high pressure high temperature gasses is used to predict their thermodynamic properties by minimizing the Gibbs free energy with respect to the concentrations of the molecular and reactive dissociation products of C,H,N,O systems in which carbon is in its oxidized form, as carbon mono- and di-oxide. The theory uses pair interactions of the exponential-six potential form. Including a three phase carbon equation of state (EOS) into such mixtures has allowed us to isolate the effect of carbon on the EOS of high temperature explosive-product-mixtures that form free carbon. A significant change must be made in the effective EOS of carbon to accommodate the non equilibrium character of the slow carbon condensation process. The results suggest a significant effect of the carbon-gas interface. The method of determining the gas phase pair interactions and the carbon component are discussed and the results compared to the data of number of explosives.

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Standard Session preferred

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