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A Complete Equation of State for Graphite-Diamond-Liquid Carbon ERIC AUROUX, OLIVIER HEUZE, CEA/DIF, B.P. 12, 91680 Bruyers-Le Châtel CEDEX, France — Many issues remain unknown about the state of carbon in detonation products, especially if it is in graphite, diamond structure or liquid or a mixture of these different phases. We propose a complete equation of state for graphite/diamond/liquid carbon based on the fundamental rules of thermodynamic equilibrium. Each phase is defined independently, the phase transition lines are obtained from the Gibbs free energy equality and provide true volume and entropy jumps, and a full description of the thermodynamic properties of binary mixtures and at the triple point. This approach, already used for other materials like Sn or Bi, is newly applied to carbon. It is particularly suited to be used with a gaseous phase to calculate the equilibrium properties of detonation products. Our model is based on classical cold/thermal contributions and heat capacities, and Grüneisen assumption. An electronic contribution is useful at high temperature. It reproduces well the experimental transition lines, triple point, and Hugoniot curve. We compare our model to Van Thiel & Ree's model, especially in the neighborhood of the mixted states where they use the Lindemann law and pressure jump. We make this comparison on the basis of very similar physical parameters and show the consequences on the properties of the phase transition.

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