Dynamic Response of HMX Through the β–δ Phase Transition

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The β–δ phase transformation in the explosive HMX has been postulated to be an important first step in the molecular decomposition of the HMX molecule [1]. The transition is also thought to be an important mechanism for the early stages of reaction. The 6–7% volume increase that occurs in the transition causes crack growth in granular HMX with an associated temperature rise [2]. Upon dynamic loading, these cracks are responsible for further heating of the HMX grains. In the present work the β–δ phase transformation is studied using a theoretical analysis based on the theory introduced by Andrews [3]. Because there is much interest in the β–δ transition as it occurs in the plastic-bonded explosive PBX-9501, an analysis based on the method of cells (MOC) that has recently been extended to include phase transformations in metal matrix composites [4] has been applied to study the HMX β–δ transformation in this explosive. Here we discuss only the HMX phase transition, however.

Details of the phase transition model are described in [4] but it is important to note that inelastic contributions come from HMX microcrack growth and plasticity [5]. A complete equation of state (EOS) is needed for both the β and δ phases. Sufficient data exists to determine the coefficients for an empirical form for the β and δ phase Gibbs free energies. Figure 1 is a plot of our calculated specific volume as a function of temperature and pressure for β and δ HMX. Also shown in Fig. 1 is the zero pressure specific volume data of Saw [6]. Along with the data of [6], the pressure-volume isotherms of Gump and Peiris [7], the zero-pressure specific heat at constant pressure of Shoemaker et al. [8], and the *ab initio* calculations of Sewell et al. [9] were used to determine the Gibbs free energy. The bend in the β–δ phase boundary (Fig. 2) is attributed to molecular decomposition and included here by making a judicious choice for the δ phase parameters in the Gibbs free energy.

The first set of simulations to be presented is that of dynamically loaded HMX. Loads are applied by specifying the strain rates. HMX is loaded compressively in one direction and tensile loaded in the two orthogonal directions. Figure 3 is a plot of the HMX volumetric strain. Abrupt jumps in the curves occur as the HMX undergoes the β–δ phase transition. Depending on the loading, HMX can undergo the expected volume increase at the transition but also volume decreases (Fig. 3). Thus, depending on the pressure reached, complex behavior can be observed.

It is known that under slow heating (cooling) rates HMX will remain in a metastable β (δ) phase far above (below) the phase boundary. It is less clear if this remains true under dynamic loading. Figure 4 shows several simulations where τ, the characteristic relaxation time that controls the rate at the transition occurs, is varied. From Fig. 4 it is clear that if the transformation rate, under dynamic loading, is sufficiently slow, the transformation will not be completed before the HMX melts (at zero pressure HMX melts at about 550 K) or reacts.

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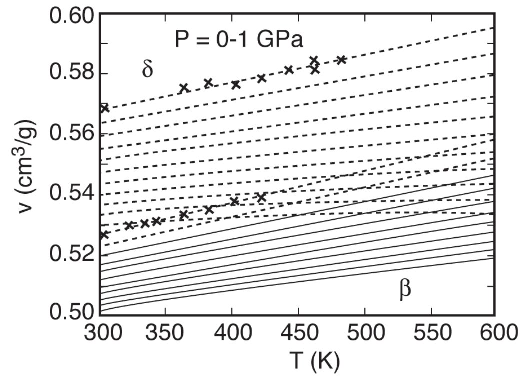

Fig. 1. *Specific volume of β and δ HMX. The points are the ambient pressure data of Saw [6]. The theoretical curves span pressures of 0 to 1 GPa.*

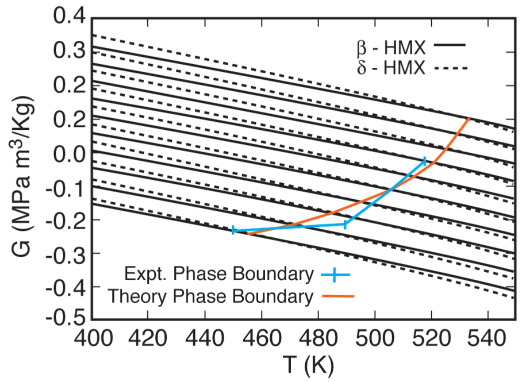

Fig. 2. *Gibbs free energies for β and δ HMX. The curve connecting the three points is an approximation to the experimental P-T phase boundary of [2] which has been overlaid on our phase diagram. The theoretical curves span pressures of 0 to 1 GPa.*

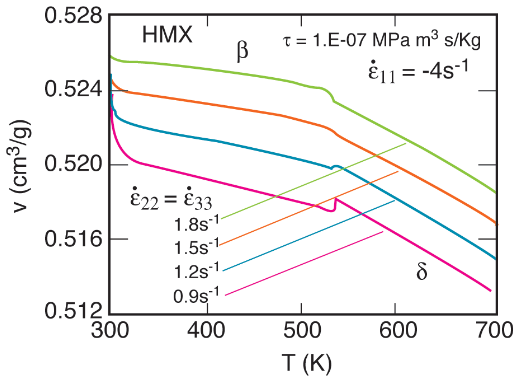

Fig. 3. *Specific volume of HMX as the β–δ phase transition is crossed.*

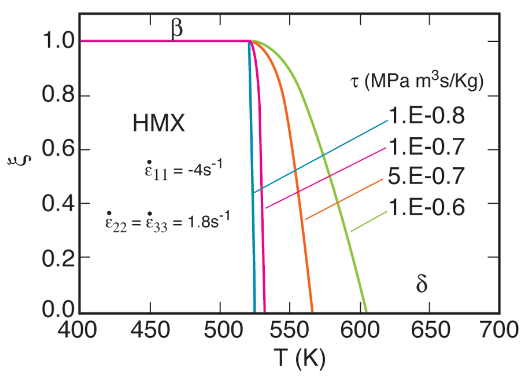

Fig. 4. *Mass fraction for the β phase for different relaxation times.*