A revised diamond–graphite transition curve

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ABSTRACT

The transition from diamond to graphite is a key equilibrium for interpreting ultrahigh-pressure metamorphic rocks. Despite widespread interest, there remain significant systematic differences between the best available experimental determinations of $P$ and $T$ (Kennedy and Kennedy 1976) and numerous thermodynamic calculations of the transition. At temperatures below 1400 K, calculated equilibrium pressures are lower than extrapolations of the experiments by as much as 5 kbar. At 3000 K, calculated pressures vary from more than 8 kbar above to almost 20 kbar below the position of the extrapolated transition. A revised curve based on a critical review of the experimental and thermodynamic data is consistent with expanded experimental brackets and the preferred calorimetric data. It is steeper than the transition proposed by Kennedy and Kennedy (1976) and previous calculations and passes through 16.2 kbar, 298 K; 33.9 kbar, 1000 K; 63.5 kbar, 2000 K; and 98.4 kbar, 3000 K.

The revised curve implies that the minimum pressure for formation of diamond-bearing crustal rocks is 3–4 kbar less than implied by extrapolation of the experiments. Because the revised transition is steeper than most previous calculations, the triple point among graphite, diamond, and liquid carbon may be as much as 40 kbar higher than previously estimated.

Keywords: Diamond, graphite, transition, equilibrium

INTRODUCTION

The diamond–graphite transition is one of the key equilibria for calibrating ultrahigh-pressure metamorphism and geodynamic processes. Despite widespread interest and numerous studies, systematic differences remain between the available experimental determinations and the locations of the transition that may be calculated from the available thermodynamic and thermophysical data. This contribution explores the source of these discrepancies and proposes a location for the transition that reconciles the experiments and the thermodynamic data.

The most widely accepted experimental determinations are those reported by Kennedy and Kennedy (1976) who summarized their experiments with a preferred linear equation (Fig. 1). They reviewed the pioneering previous work (Bundy et al. 1961; Strong and Hanneman 1967; Strong and Chrenko 1971), but noted that those experiments were not specifically designed to determine the pressure of the transition, and may have had significant systematic errors in the pressure calibrations. Published experimental work since 1976 has focused primarily on the synthesis of diamond in various catalytic media, as well as on novel forms and phase equilibria of carbon at several hundreds of kbar and temperatures approaching the triple point (e.g., Bundy et al. 1996; Akaishi et al. 2001; Dobrzhinetskaya et al. 2004). Consequently, it appears that the experimental determinations of Kennedy and Kennedy (1976) remain the best available.

With all that we have learned about the need for internally consistent thermodynamic data sets (e.g., Berman 1988; Holland and Powell 1998), it might be expected that the location of the transition calculated using commonly cited calorimetric data would be different than the experimentally determined location (Fig. 1; Table 1). Assuming constant molar volumes (298 K, 1 bar) of diamond and graphite yields differences of 6–10 kbar.