

Appendix Materials for “A revised diamond-graphite transition curve”

HOWARD W. DAY

deposit number AM-12-001

Jan 2012 issue of American Mineralogist, pages 52-62,

DOI: <http://dx.doi.org/10.2138/am.2011.3763>

Figure A1. Deviations of measured graphite heat capacity from the selected values of Chase (1998). Abbreviations: CM, Cezairliyan and Müller (1985); CR, Cezairliyan and Righini (1975, po: poco graphite; py: pyrolytic graphite); M, Macdonald (1965); WI, West and Ishihara (1965).

Figure A2. Heat capacity of graphite versus temperature. The smoothed data from Chase et al. (1998) are constrained by measurements up to 3000 K. Abbreviations: C, Chase (1998); G, Gustafson (1986); H&P, Holland and Powell (1998).

Figure A3. Deviations of graphite heat capacity functions from the selected values of Chase (1998). Abbreviations: E, Evans (1960); G, Gustafson (1986); Gl, Glusko et al. (1979); H, Hultgren et al. (1973); H&P, Holland and Powell (1998); RH, Robie and Hemingway (1995).

Figure A4. Heat capacity of diamond versus temperature. Measurements of the heat capacity are restricted to temperatures below 1073 K (Victor, 1962). Abbreviations: R&W, Reeber and Wang (1996, $B_0=5560$); V, Victor (1962); others as in Figure A3.

Figure A5. Deviations of diamond heat capacity functions from the smoothed values of Victor (1962). R&W, Reeber and Wang (1996, $B_0=5560$ or 4400); others as in Figs. A3, A4.

Figure A6. Compression of graphite versus pressure at 293 K. Abbreviations: B, Bridgeman (1945,1948); G, Gustafson,(1986); H, Hanfland et al., 1989; H&P, Holland and Powell (1998); L&D, Lynch & Drickamer (1966).

Figure A7. Compression of diamond versus pressure. Temperature was not specified but is presumed to be 293 K, as for graphite (Lynch and Drickamer, 1966). Abbreviations: D, Drickamer (1966); L&D, Lynch and Drickamer, 1966; OC03, Occelli et al., 2003.

Figure A8. Thermal expansion of graphite. Abbreviations: G, Gustafson (1986); H&P, Holland and Powell (1998); N&R, Nelson and Riley, 1945; T, Touloukian et al. (1977).

Figure A9. Thermal expansion coefficient of graphite versus temperature. Abbreviations as in Fig. A8.

Figure A10. Thermal expansion of diamond. Abbreviations: R&W, Reeber and Wang (1996), others as in Figure A8.

Figure A11. Thermal expansion coefficient of diamond versus temperature. Abbreviations as in Fig. A10, A8.

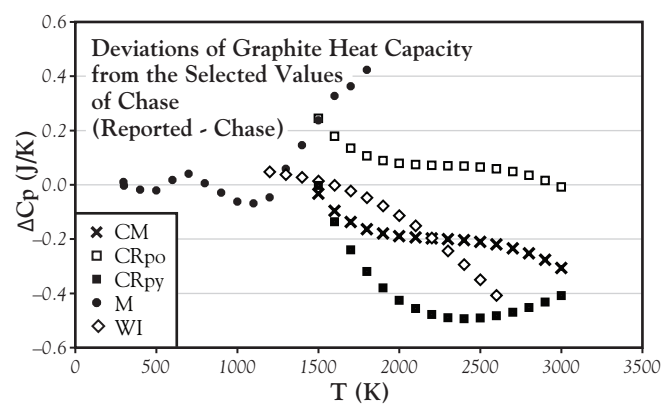


Fig A1

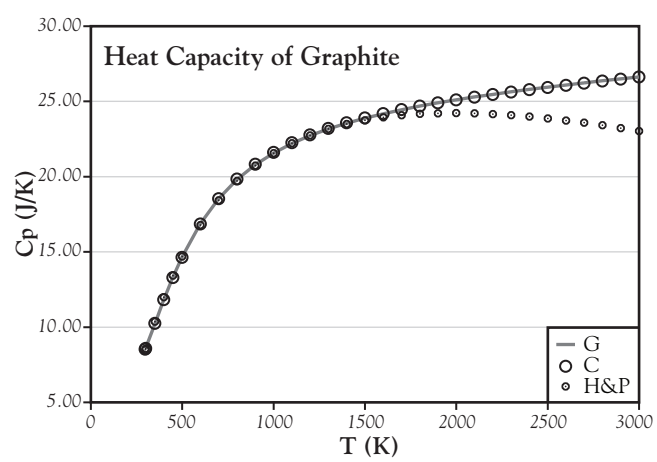


Fig A2

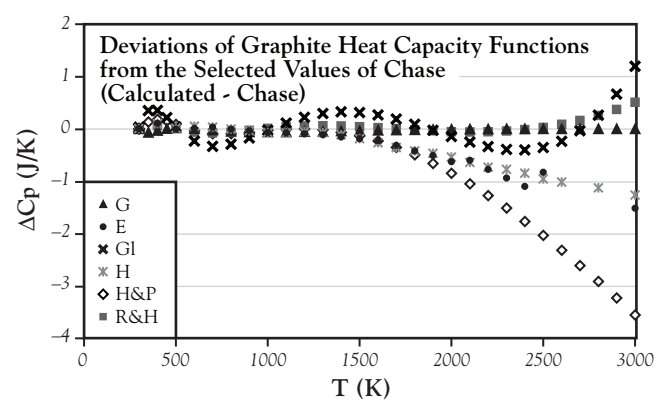


Fig A3

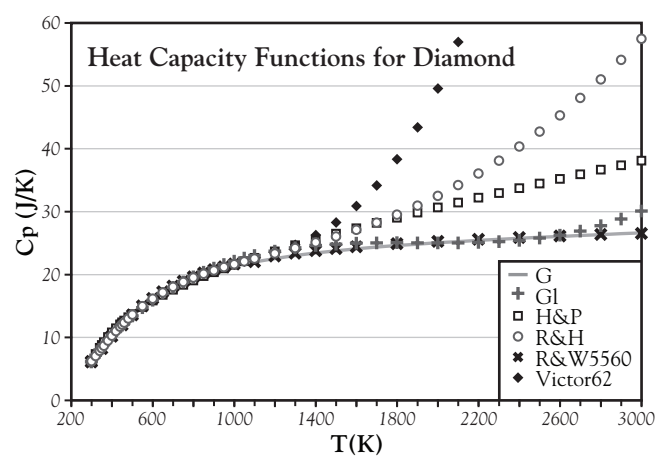


Fig A4

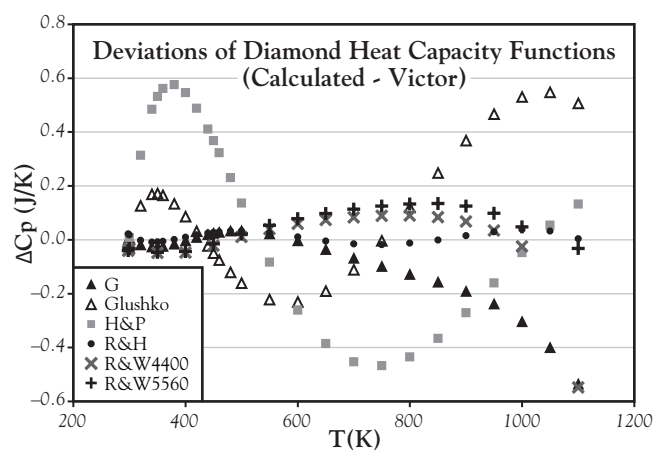


Fig A5

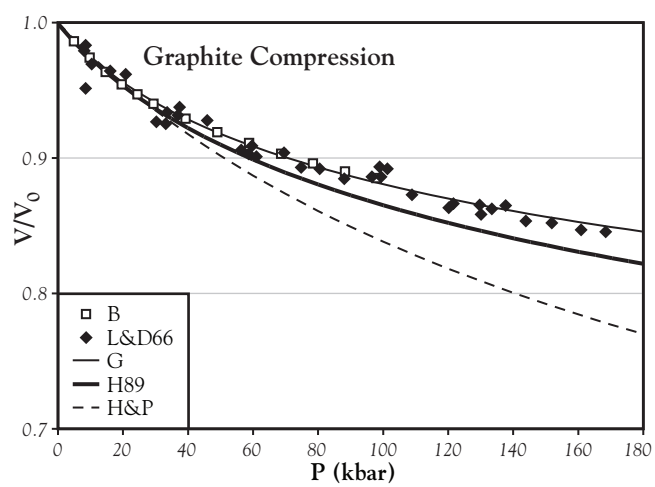


Fig A6

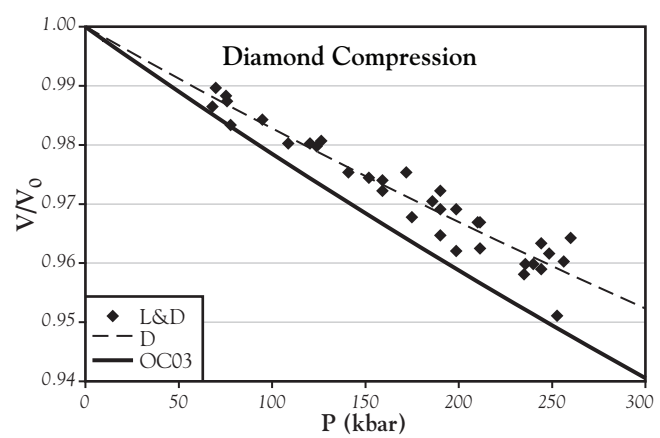


Fig A7

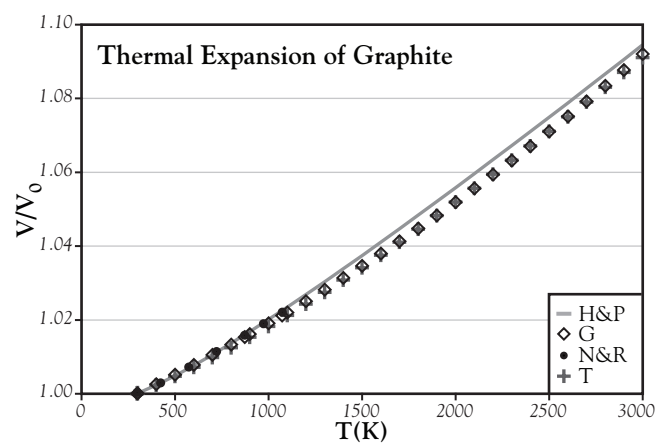


Fig A8

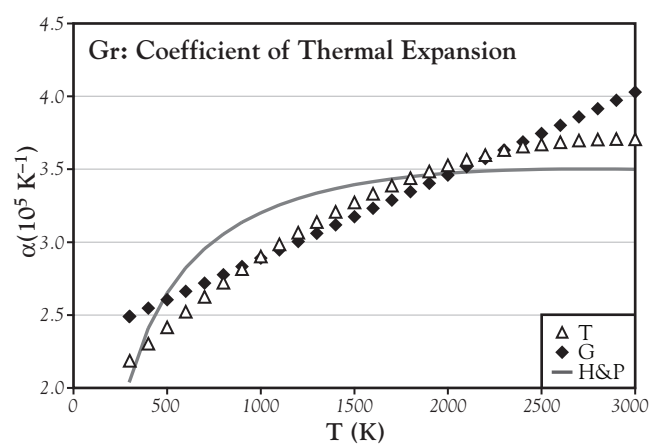


Fig A9

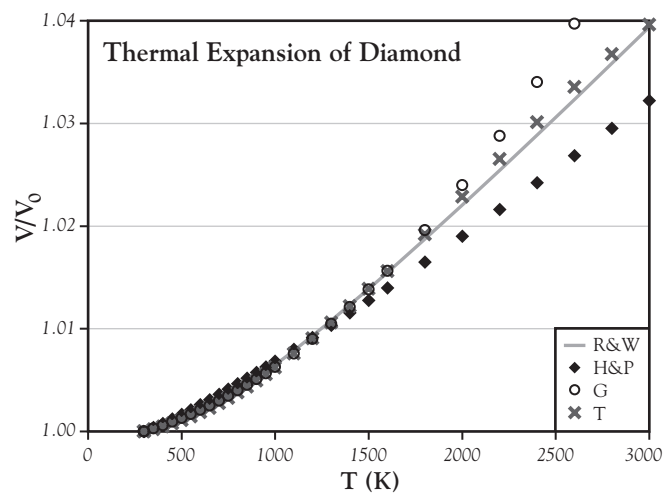


Fig A10

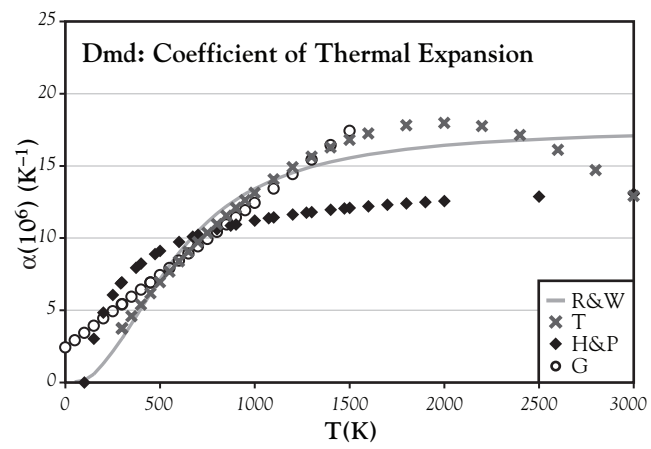


Fig A11

Table A1. Entropy and high temperature heat capacity of graphite.

Source		$S^0(298,1)$ 2σ (J/mol-K)		References Cited	
				S & Low-T C_p	High-T C_p
Holland&Powell*	1998	5.85		*Robie&Hemingway95	Robie&Hemingway95
		none			
Chase (JANAF)	1998	5.74		Cox71	MacDonald65
		0.21			West&Ishihara65
					Cezairliyan&Righini75
					**Cezairliyan&McClure77
Robie&Hemingway	1995	5.74		Cox89	Cox89
		0.10			
Cox et al. (CODATA)	1989	5.74		DesSorbo55	Chase82
		0.10		DeSorbo&Nichols58	
				DeSorbo&Tyler53	
Gustafson	1986	5.74		Chase82	Chase82
		0.21			
Chase et al. (JANAF)	1982	5.74		Cox71	McDonald65
		0.21			West&Ishihara65
Berman	1979	5.72		Berman65	Berman65
		0.02			
Robie et al.	1978	5.74		Hultgren73	Hultgren73
		0.01			
Hultgren et al.	1973	5.73		DeSorbo&Nichols58	Evans60
		0.04		DeSorbo&Tyler53	
				Evans64	
				Jacobs&Park34	
				Keesome&Pearlman55	
				van de Hoeven&Keesom63	
Cox et al. (CODATA)	1971	5.74		DeSorbo&Tyler53	
		0.12			
Berman	1965	5.720		DeSorbo&Tyler53	Kelley60
		0.02		Bergenslid54	Lucks60
				DeSorbo&Nichols58	Rasor&McClelland60
				Bowman&Krumhansl,1958	
Evans	1964	5.74		none	
Evans	1960	5.74		none	none
Berman&Simon	1955	5.73		DeSorbo&Tyler53	Kelley49
		0.02		Bergenslid54	
DeSorbo&Tyler***	1953	5.74			
		0.02			

* value adjusted from that reported by reference

** Does not contain cited information

*** 298.16 K

Table A2. Entropy, enthalpy of formation, and heat capacity of diamond.

Source		$S^0(298,1)$	ΔH_f	References cited		
		J/mol-K	kJ/mol	S & Lo-T C_p	H	High-T C_p
Holland&Powell	1998	2.30	2.07 0.07	*Robie&Hemingway95	derived	Robie&Hemingway95
Robie&Hemingway	1995	2.38 0.2	1.900 0.000	Wagman82	Wagman82	Wagman82?
Gustafson	1986	2.36	1.895	from equation Hultgren73	from equation Hultgren73	Hultgren73
Wagman et al.	1982	2.377	1.895	none	none	none
Berman	1979	2.356 0.02	1.872 0.075	Berman65	Hawtin66	
Robie et al	1978	2.38 0.01	1.895 0.042	Hultgren73	Hawtin66	Hultgren73
Hultgren et al.	1973	2.38 0.04	1.895	Evans64	Evans64	Victor62
Wagman et al.	1973	2.38 0.04	1.895	Desnoyers&Morrison58 DeSorbo53	Evans,1964	Victor62
Hawtin et al.	1966		1.872 0.074			
Berman	1965	2.356 0.02	1.895 0.084	DeSorbo53 Berman&Poulter53 Burk&Friedburg58 Desnoyers&Morrison58	Prosen44	Victor62
Evans	1964	2.377	1.897	none	none	
Berman&Simon**	1955	2.377 0.020	1.895	DeSorbo53 Berman&Poulter53	Prosen44	Kelley49
DeSorbo	1953	2.38 0.02				
Prosen et al.**	1944		1.896 0.085		Dewey&Harper38 Jessup38 Prosen&Rossini44	

* value adjusted from that reported by reference

** 298.16 K

Table A4. Molar volume, bulk modulus and thermal expansion of graphite.

		$V(298,1)$	B_0^*	n^{**}	References cited		
		2σ (cm ³)	(kbar)		V	B_0	α^{***}
Holland&Powell	1998	5.30	390	4	Robie& Hemingway95	Birch66	Skinner66
		none					
Robie&Hemingway	1995	5.298			Robie67 (?)		
		0.001					
Hanfland et al.	1989	5.287	338	8.9			
		0.003	3	0.1			
Gustafson	1986	5.297	333	12	Berman&Simon55	Lynch&Drickamer66	Nelson&Riley45
		none					Bacon50
							Touloukian77
Berman	1979	5.299	337	12.2	Berman65	Drickamer et al.66	Berman65
		0.001					
Robie et al.	1978	5.298			Robie67 (?)		
		0.001					
Robie et al.	1967	5.2982			Nelson&Riley45		
		0.0009					
Drickamer et al.	1966		337	12.2		Lynch&Drickamer66	
Lynch&Drickamer	1966						
Birch	1966		333			Richards15	
Skinner	1966						Nelson&Riley45
Berman	1965	5.299	379		Berman&Simon55	Bridgman45,48	Nelson&Riley45
					Implied		Bacon50
Berman&Simon	1955	5.299			Nelson&Riley45	Bridgman45,48	Nelson&Riley45
					Bacon50		Bacon50
Nelson&Riley	1945	not reported					

* Initial bulk modulus.

**Pressure derivative of bulk modulus.

***Coefficient of thermal expansion.

Table A5. Molar volume bulk modulus, and thermal expansion of diamond.

Reference		V(298,1) 2σ	B ₀ *	n**	References Cited		
		cm3	kbar		V	B ₀	α***
Occelli et al.	2003	3.4170 0.0008	4460 10	3.2			
Holland&Powell	1998	3.42	5800	4	Robie&Hemingway95	Birch66?	Skinner,66
Reeber&Wang	1996	3.4166 0.0003			calculated using cell volume Tu32 Straumanis&Aka51 Thewlis&Davey56 Skinner57 Hom75 Robie67?	Table IV Equation	
Robie&Hemingway	1995	3.417 0.001					
Gustafson	1986	3.416	5882	5	from equation Berman&Simon55	Lynch&Drickamer66	Touloukian77
Berman	1979	3.4165	4400		Berman65 Mykolajewycz65	McSkimin&Bond57 McSkimin&Andreatch72 McSkimin et al.72 Grimsditch&Ramdas75	Berman65 Wright66 Slack&Bartram75
Robie et al.	1978	3.417 0.001			Robie67?		
Robie et al.	1967	3.4166 0.0003			Parrish60 Mykolajewycz64 Skinner57		
Drickamer et al.	1966		5560	4		Lynch&Drickamer66	
Lynch&Drickamer	1966		6250				
Birch	1966		5556 #4425 #5747			Adams21,23 McSkimin&Bond57 Bhagavantam& Bhimasenachar44	
Skinner	1966						Mauer&Bolz57a

Berman	1965	3.4165	5448	Straumanis&Aka51 Thewlis&Davey56	Bridgman45? No value reported	Skinner57 Thewlis&Davey56 Skinner57 Kaiser&Bond59 Parrish60 only supplement found
Mauer&Bolz	1957					
Skinner	1957	3.4168				
		0.0001				
Berman&Simon	1955	3.4165	not reported	Straumanis&Aka51 Bearden38 Tu32	Bridgeman45	Thewlis&Davey56?

*Initial bulk modulus

** Pressure derivative of bulk
modulus

***Coefficient of thermal expansion

#Calculated from elastic constants
