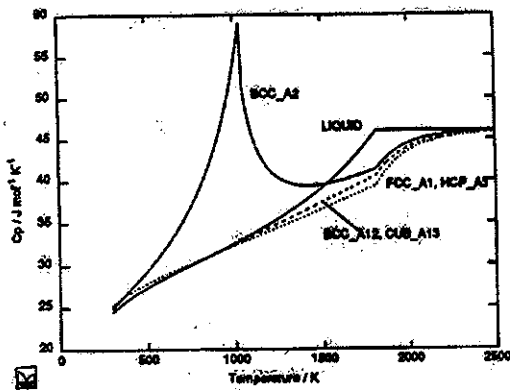
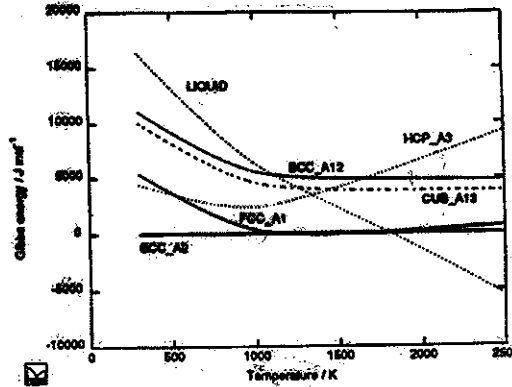


## Termodynamické charakteristiky a fázový p.t - diagram železa

Závislosti tepelných kapacit a Gibbsových energií na teplotě pro různé fázové modifikace Fe:  
při  $p=101325\text{Pa}$

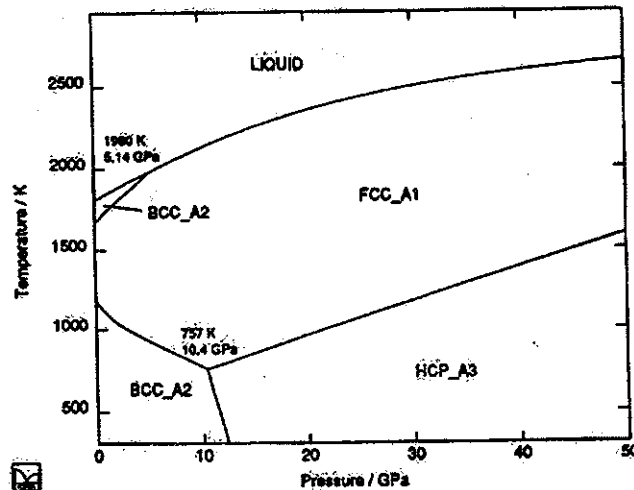


Heat capacity of Fe



Gibbs energy of phases of Fe relative to BCC\_A2

Fázový diagram Fe:



P-T phase diagram for Fe

Data for Fe relative to paramagnetic BCC\_A2

BCC\_A2

$T_c = 1043$        $B_0 = 2.22$   
 $A = 7.042095E-6$        $a_0 = 2.3987E-5$        $a_1 = 2.569E-8$   
 $K_0 = 5.965E-12$        $K_1 = 6.5152E-17$        $n = 4.7041$

Gmag + Gpres

(298.15 < T < 6000.00)

Data for Eu relative to BCC\_A2

LIQUID

8382.505 - 7.175215 T  
 20837.691 - 239.524939 T + 37.192045 T ln(T) - 46.128567E-3 T<sup>2</sup> + 9.459498E-6 T<sup>3</sup> - 749625 T<sup>-1</sup> (298.15 < T < 400.00)  
 280532.835 - 1999.21579 T + 271.2408609 T ln(T) - 114.530917E-3 T<sup>2</sup> + 8.809866E-6 T<sup>3</sup> - 48455305 T<sup>-1</sup> (400.00 < T < 1095.00)

$$G = a + bT + cT \ln(T) + \sum dT^n \quad S = -\left(\frac{\partial G}{\partial T}\right)_P \quad (1095.00 < T < 1900.00)$$

Fe

$$H = G + TS, \quad C_p = \left(\frac{\partial H}{\partial T}\right)_P$$

Source of data:

A Fernandez Guillemet, P Gustafson, High Temp. - High Press., 1985, 16, 591-610. [BCC\_A2, FCC\_A1, HCP\_A3, LIQUID]  
 Weiming Huang, TRITA-MAC-0388 [BCC\_A12, CUB\_A13].

Data for Fe in the form of G-HSER

BCC\_A2

T<sub>C</sub> = 1043                      B<sub>0</sub> = 2.22  
 A = 7.042095E-6              a<sub>0</sub> = 2.3987E-5              a<sub>1</sub> = 2.569E-8  
 K<sub>0</sub> = 5.965E-12              K<sub>1</sub> = 6.5152E-17              n = 4.7041

\* 1225.7 + 124.134 T - 23.5143 T ln(T) - 0.00439752 T<sup>2</sup> - 5.89269E-8 T<sup>3</sup> + 77358.5 T<sup>-1</sup> + Gmag + Gpres (298.15 < T < 1811.00)  
 -25383.581 + 299.31255 T - 46.0 T ln(T) + 2.2960305E31 T<sup>9</sup> + Gmag + Gpres (1811.00 < T < 6000.00)

FCC\_A1

T<sub>N</sub> = 67                      B<sub>0</sub> = 0.7  
 A = 6.688726E-6              a<sub>0</sub> = 7.3097E-5  
 K<sub>0</sub> = 6.2951E-12              K<sub>1</sub> = 6.5152E-17              n = 5.1665

-236.7 + 132.416 T - 24.6643 T ln(T) - 0.00375752 T<sup>2</sup> - 5.89269E-8 T<sup>3</sup> + 77358.5 T<sup>-1</sup> + Gmag + Gpres (298.15 < T < 1811.00)  
 -27097.396 + 300.25256 T - 46.0 T ln(T) + 2.78854E31 T<sup>9</sup> + Gmag + Gpres (1811.00 < T < 6000.00)

HCP\_A3

A = 6.59121E-6              a<sub>0</sub> = 7.3646E-5  
 K<sub>0</sub> = 6.2951E-12              K<sub>1</sub> = 6.5152E-17              n = 5.1665

-2480.08 + 136.725 T - 24.6643 T ln(T) - 0.00375752 T<sup>2</sup> - 5.89269E-8 T<sup>3</sup> + 77358.5 T<sup>-1</sup> + Gpres (298.15 < T < 1811.00)  
 -29340.78 + 304.56206 T - 46.0 T ln(T) + 2.78854E31 T<sup>9</sup> + Gpres (1811.00 < T < 6000.00)

LIQUID

A = 6.62574E-6              a<sub>0</sub> = 10.7895E-5              a<sub>2</sub> = -25.79493  
 K<sub>0</sub> = 0.75475E-12              K<sub>1</sub> = 485.09E-17              n = 6.59834

\* 13265.87 + 117.57557 T - 23.5143 T ln(T) - 0.00439752 T<sup>2</sup> - 5.89269E-8 T<sup>3</sup> + 77358.5 T<sup>-1</sup> - 3.6751551E-21 T<sup>7</sup> + Gpres (298.15 < T < 1811.00)  
 -10838.83 + 291.302 T - 46.0 T ln(T) + Gpres (1811.00 < T < 6000.00)

BCC\_A12

5970.7 + 124.134 T - 23.5143 T ln(T) - 0.00439752 T<sup>2</sup> - 5.89269E-8 T<sup>3</sup> + 77358.5 T<sup>-1</sup> (298.15 < T < 1811.00)  
 -20638.581 + 299.31255 T - 46.0 T ln(T) + 2.2960305E31 T<sup>9</sup> (1811.00 < T < 6000.00)

CUB\_A13

4970.7 + 124.134 T - 23.5143 T ln(T) - 0.00439752 T<sup>2</sup> - 5.89269E-8 T<sup>3</sup> + 77358.5 T<sup>-1</sup> (298.15 < T < 1811.00)  
 -21638.581 + 299.31255 T - 46.0 T ln(T) + 2.2960305E31 T<sup>9</sup> (1811.00 < T < 6000.00)

## Sbírkový dat

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- HULTGREN R. a kol.: *Selected Values of The Thermodynamic Properties of The Elements*. ASM, Ohio 1973

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- REID R.C., PRAUSNITZ J.M., SHERWOOD T.K.: *The Properties of Gases and Liquids*.  
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- HALA E., WICKTERLE I., POLAK J., BOUBLÍK T.: *Vapour-Liquid Equilibrium Data at Normal Pressures*. Pergamon Press, Oxford 1968.  
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Parametrizace: WILLIAMS R.O.: CALPHAD 15 (1991), 1.

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Další: INT. CRIT. TABLES  
LANDOLT, BERNSTEIN

• DATABASE: THERMOCALC, MTDATA ... PD.