PVT EoS of Cr_2O_3 (eskolaite): implication for phase boundary calculation in knorringite system

A. M. DYMSHITS [1]*, I.S. SHARYGIN [1], K. D. LITASOV [1,2], A. SHATSKIY [1,2], S.V. RASHCHENKO [1,2]

[1] Sobolev Institute of Geology and Mineralogy, Novosibirsk 630090, Russia (*a.dymshits@gmail.com)

[2] Novosibirsk State University, Novosibirsk, 630090, Russia

Synchrotron X-ray diffraction study of Cr_2O_3 (eskolaite) has been carried out in a Kawai-type multi-anvil apparatus (Spring-8, Japan) up to 15 GPa and 1873 K. Fitting the BM EoS with the present data yielded: $K_{0,T0}$, = 206 (4) GPa; $K'_{0,T}$ = 4.4 (8); $\partial K_{0,T}/\partial T$ = □0.037 (6) GPa K$^{□1}$; a = 2.98 (14) × 10^{-5} K^{-1} and b = 0.47 (28) × 10$^{□8}$ K$^{□2}$, where $\alpha_{0,T} = a + bT$. Fitting the MGD EoS yielded: $K_{0,T0}$ = 204.7 GPa, $K'_{0,T}$ = 4.0, γ_0 = 1.42, q = 1.82. The thermoelastic parameters indicate that Cr_2O_3 undergoes near isotropic compression at room and high temperatures up to 15 GPa. Cr_2O_3 is shown to be stable in this pressure range and adopts the corundum type structure. Using obtained thermoelastic parameters we calculated the reaction boundary of knorringite formation from enstatite and Cr_2O_3 (Fig.1) [1,2,3]. The Clapeyron slope (dP/dT -0.014 GPa/K) was found to be consistent with experiments [2].

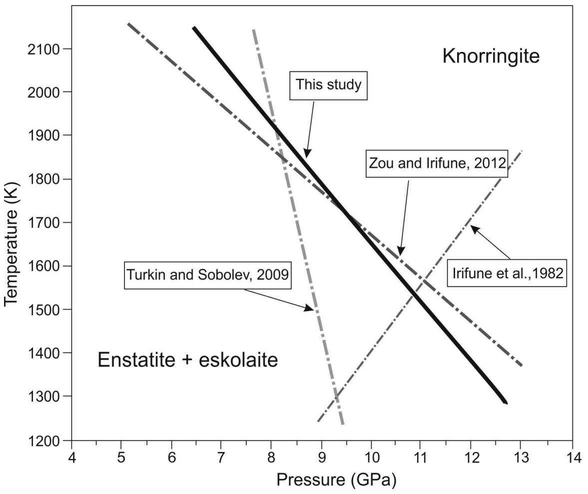

Figure 1: Phase relations in the $Mg_3Cr_2Si_3O_{12}$ system based on thermodynamic calculations.

[1] Turkin and Sobolev (2009) *GeolGeophys* **50**, 1169-1182. [2] Zou and Irifune (2012) *JMPS* **107**, 197-205. [3] Irifune et al., (1982) *PEPI* **27**, 263-272.

The study was supported: Ministry of Education and Science of Russian Federation (project No 14.B25.31.0032) and RFBR (grants 14-05-00957 and 15-35-20556).