Correlation between crystallization pressure and structural parameters of phengites

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ABSTRACT

Linear correlations of ln P vs. the thickness, t, of the TOT mica module and vs. the ditrigonal distortion, α, have been established by analyzing a population of 43 natural phengites for which estimates of the crystallization pressure P independent of the Si content are available. Synthetic phengites are not included because they behave as a separate population. The equations for the resultant regression lines are ln P = −0.35(3)α + 5.0(3) (R = 0.90, 26 observations) and ln P = −29(2)t + 293(22) (R = 0.90, 43 observations). These linear correlations are evidence of the links involving P, chemical composition, structural parameter c (i.e., t), and α. In turn, there is a linear correlation between t and α: t = 0.0110(9)α + 9.859(7) (R = 0.92, 26 observations). The linear correlations of ln P, t, and α vs. Si content have equations: ln P = 4.2(4)Si − 12(1) (R = 0.86, 43 observations), t = −0.13(1)Si + 10.37(4) (R = 0.87, 43 observations), and α = −12.7(9)Si + 50(3) (R = 0.94, 26 observations). The observed dispersion of the data are mainly due to the uncertainty in the pressures estimated from mineral assemblages. The possibility of calculating P from only a measurement of c neither overcomes this type of uncertainty nor pretends to be competitive with petrologic geobarometers, but is does open the possibility of estimating the crystallization pressure of nanoscale phengite relics (e.g., by transmission electron diffraction).

Keywords: Phengites, crystallization pressure, pressure-structure correlation, ditrigonal distortion, mica module thickness

INTRODUCTION

According to Rieder et al. (1998), phengite is a series name for solid solutions of the dioctahedral micas muscovite, aluminocladonite, and celadonite. The phengites discussed in this paper do not include celadonites and belong to the series with composition K[Al₁₋ₓ(Mg, Fe²⁺)ₓ][Al₁₋ₓ,Siₓ, O₆)(OH)₂, ignoring minor substitutions.

The polytypes 3T and 2M₁ that occur among phengites differ not only in the geometrical stacking of the tetrahedral-octahedral-tetrahedral (TOT) layer, but also in the occupancy of the two octahedral sites of the O sheet, which are equivalent in 2M₁ (space group C2/c) and independent in 3T (space group P3₁2₁). As a direct consequence, the two polytypes, not differing only in the stacking of the TOT layer, should be considered just polymorphs. The higher degree of structural freedom (i.e., two independent octahedral sites) in 3T phengites has been used to explain the common occurrence of this polymorph relative to the 2M₁ variety at high pressure. The occurrence may also be a consequence of a 2M₁ → 3T transition suggested by Sassiet al. (1994) for increasing pressure at subduction conditions. The argument that structural flexibility allows cation ordering has been discussed in particular by Pavese et al. (1997, 1999, 2000, 2001, 2003), who reported some degree of octahedral cation ordering for several 3T-phengite samples investigated by neutron diffraction.

The Si content of phengites increases with pressure (Massonne and Schreyer 1986, 1987, 1989) and strongly affects the values of both the c cell parameter and the ditrigonal rotation, α. The latter is a measure of the deviation from the ideal hexagonal symmetry of the T sheet (Fig. 1), and is defined as 2α = Σᵢ=1₆(|120 − φᵢ|)/6, where φᵢ are the internal angles of the ideally hexagonal ring in the T sheet. The ditrigonal rotation is one of the adjustable parameters used by nature to fit the dimensions at the interface between T and O sheets, complementing the dimensional adjustment that can be achieved via the so-called celadonite substitution (Si + Mg → ³⁰Al + ³¹Al). In their Figure 13, Ferraris and Ivaldi (2002) showed a decrease of both c and α parameters with increasing of Si: the smaller the α, the more hexagonal the T sheet is, and the better the interlayer cation can sink within the sheet itself (i.e., the c parameter shortens).

In this paper, we demonstrate that a meaningful direct correlation can be established between the estimated crystallization pressure of a phengite and the c and α parameters.

DATA FROM THE LITERATURE

Due to the petrologic importance of the celadonitic substitution as one of the most effective geobarometers available for a variety...