Supplementary Table 4

Estimation of Fe_2O_3 and FeO contents in mica from EMPA data in Xihuashan

The Fe_2O_3 and FeO contents in micas are estimated according to the method proposed by Lin and Peng (1994). Micas have an ideal formula $X\{Y_{2\text{-}3}[Z_4O_{10}](F,OH)_2\}$, which means that the cation total per formula unit (pfu) is between 7 and 8 when the anion total is 11 (2F, 2Cl or 2OH = O). When assuming that all the iron is present as Fe^{3+}, the calculated cation total pfu will be the lower limit of value (termed as F_1). When assuming that all the iron is present as Fe^{2+}, the calculated cation total pfu will be the upper limit of value (termed as F_2). At first, an initial correction number (C_0) is calculated based on the iteration method using F_1 and F_2 values. Then a new correction number (C_1) is calculated based on iteration method using F_2 and C_0 (instead of F_1). At last, we can estimate the FeO and Fe_2O_3 in micas based on the new correction number (C_1). The detail calculation steps of the cation total is as follows (Table S1):

Step 1: Read the oxide contents (wt%) from the EPMA data.

Step 2: Calculate the cation total (F_1) pfu assuming that all the iron is present as Fe^{3+}.

Step 3: Calculate the cation total (F_2) pfu assuming that all the iron is present as Fe^{2+}.

Step 4: Calculate the initial correct number of cations (C_0) based on F_1 and F_2:

$$C_0 = (F_2 \times (8 - F_1) + F_1 \times (8 - F_2)) / ((8 - F_1) + (8 - F_2))$$

Step 5: Calculate the new correct number of cations (C_1) based on F_2 and C_0:

$$C_1 = (F_2 \times (8 - C_0) + C_0 \times (8 - F_2)) / ((8 - C_0) + (8 - F_2))$$

Step 6: Estimate the FeO and Fe_2O_3 in micas according to the following equations:

$$\frac{2m_{Fe2O3}}{M_{Fe2O3}} \times M_{FeO} + m_{\mathrm{FeO}} = m_{\mathrm{FeOT}} \quad (1)$$

$$\frac{11}{\sum N_{Anion}} = \frac{C_1}{\sum N_{Cation}} \quad (2)$$

$$\sum N_{Anion} = \frac{2m_{SiO2}}{M_{SiO2}} + \frac{2m_{TiO2}}{M_{TiO2}} + \frac{3m_{Al2O3}}{M_{Al2O3}} + \frac{3m_{Fe2O3}}{M_{Fe2O3}} + \frac{m_{\mathrm{FeO}}}{M_{FeO}} + \cdots + \frac{m_{K2O}}{M_{K2O}} \quad (3)$$

$$\sum N_{Cation} = \frac{m_{SiO2}}{M_{SiO2}} + \frac{m_{TiO2}}{M_{TiO2}} + \frac{2m_{Al2O3}}{M_{Al2O3}} + \frac{2m_{Fe2O3}}{M_{Fe2O3}} + \frac{m_{\mathrm{FeO}}}{M_{FeO}} + \cdots + \frac{2m_{K2O}}{M_{K2O}} \quad (4)$$

Equation (1) can be transformed into the following equation:

$$\frac{m_{\mathrm{FeOT}}}{M_{FeO}} = \frac{2m_{Fe2O3}}{M_{Fe2O3}} + \frac{m_{\mathrm{FeO}}}{M_{FeO}} \quad (5)$$

By taking Equation (1) and (3)~(5) into (2), we can have the following equation:

$$m_{Fe2O3} = \frac{11M(FeO)\sum N_{Cation} - M(FeO) \times A_0 C_1 - m_{\mathrm{FeOT}} \times C_1}{M(FeO) \times C_1} \times \mathrm{M}(Fe_2O_3) \quad (6)$$

where m and M represent weight percent (wt.%) and relative molecular mass of corresponding component, respectively. A_0 represents $\sum N_{Anion}$ except for Fe.

In most cases, the method described above yields Fe_2O_3 and FeO contents consistent with wet chemical analysis (Table S1).

Reference

Lin, W.W., and Peng, L.J. (1994) The estimation of Fe^{3+} and Fe^{2+} contents in amphibole and biotite from EPMA data. Journal of Changchun University of Science and Technology, 24(2), 155–162 (in Chinese with English abstract).

Table S1. The case of estimation of Fe_2O_3 and FeO in micas

Steps		SiO_2	TiO_2	Al_2O_3	FeO_T	MnO	MgO	CaO	Na_2O	K_2O	Total
1	Content (wt%)	38.30	3.60	13.99	23.82	0.09	7.96	0.90	0.50	8.31	97.47
2	Cation total pfu at Fe^{3+}	2.7124	0.1918	1.1677	1.4109	0.0054	0.8404	0.0683	0.0687	0.7508	7.2163
3	Cation total pfu at Fe^{2+}	2.8982	0.2049	1.2477	1.5076	0.0058	0.8980	0.0730	0.0734	0.8022	7.7108
4	Calculate the initial correct number of cations (C_0)							C_0 = 7.5775			
5	Calculate the new correct number of cations (C_1)							C_1 = 7.6316			
6	Estimate the FeO and Fe_2O_3							Fe_2O_3 = 4.01 wt%, FeO = 20.21 wt%			
Comparison with the wet chemical analysis data								Fe_2O_3 = 3.98 wt%, FeO = 20.24 wt%			