

Temporal evolution of proto-Izu–Bonin–Mariana arc volcanism over 10 Ma: Constraints from statistical analysis of melt inclusion compositions

Supplementary Appendix

1. Comparison of analytical results with EPMA and SIMS

We analysed 47 melt inclusions for their volatiles (H_2O , S, F and Cl) and P_2O_5 content using Secondary Ion Mass Spectrometry (SIMS) to extend the dataset of Brandl *et al.* (2017) and better constrain the temporal evolution of the proto-IBM arc volcanism. Among the elements analysed with SIMS, P_2O_5 , Cl and S have already been analysed with EPMA (Brandl *et al.*, 2017). A correlation of the content of these elements acquired with EPMA and SIMS is compared in Fig. S1 to check the consistency of the analytical data by two methods. The P_2O_5 and Cl contents in the melt inclusions determined by the two methods are consistent (Figs. S1a and b). Considering that the reference glasses for SIMS analysis have a range of Cl content from 12 to 2833 ppm, extrapolating the calibration line of Cl toward >8000 ppm may not be reasonable. We consider the analytical results with EPMA to be more reliable for high-Cl melt inclusions (> 8000 ppm) than those with SIMS, because we used either scapolite (1.43 wt % Cl) or tugtupite (7.57 wt % Cl) as the Cl standards for analysis with EPMA. In this study, we thus use the Cl data analysed with EPMA for three high-Cl melt inclusions (>8000 ppm). The S contents are consistent between the two methods when $\text{S} \leq 1000$ ppm; however, for $\text{S} \geq 1000$ ppm, the S content analysed with SIMS is systematically higher (Fig. S1c). One possible explanation is that the analysis of melt inclusions with EPMA underestimates the S content. Some melt inclusions have been analysed by assuming that S dissolves as sulphate in oxidised arc melts (e.g. Carrol & Rutherford, 1988; Wallace & Carmichael, 1992, 1994); we analysed S at a fixed peak position of SrSO_4 as the S standard. This analytical technique could underestimate the S content if some amount of S is present in melt as sulphide. In this study, we thus used the S content analysed with SIMS.

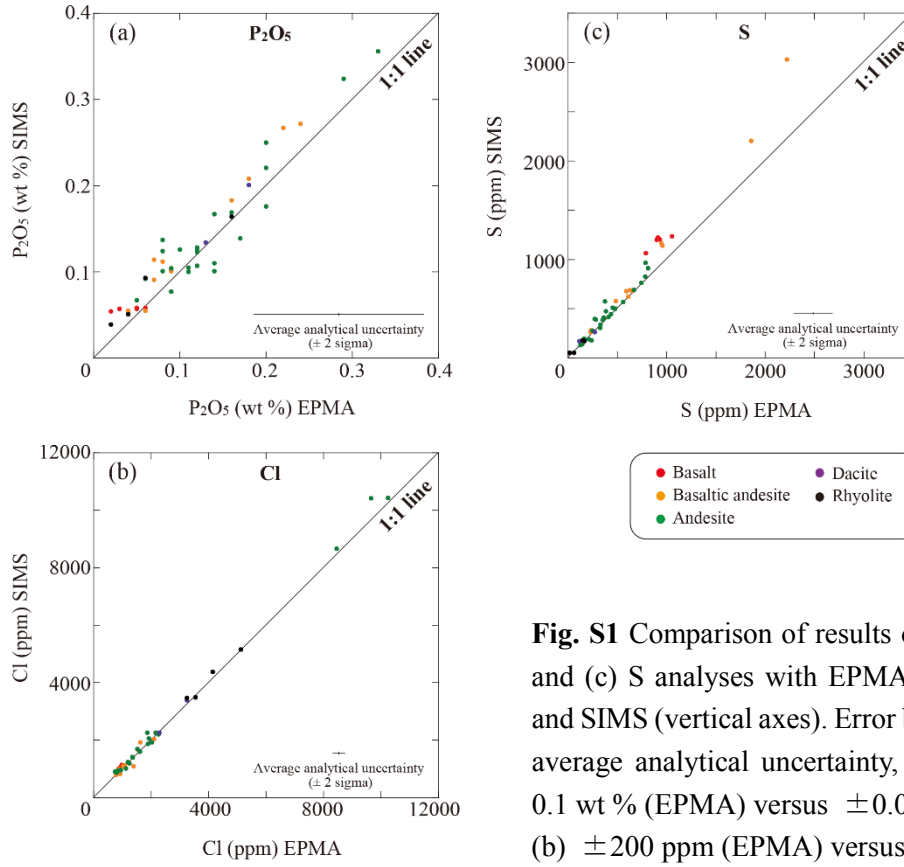


Fig. S1 Comparison of results of (a) P₂O₅, (b) Cl and (c) S analyses with EPMA (horizontal axes) and SIMS (vertical axes). Error bars (2 σ) represent average analytical uncertainty, which are (a) ± 0.1 wt % (EPMA) versus ± 0.003 wt % for P₂O₅, (b) ± 200 ppm (EPMA) versus ± 4 ppm (SIMS) for Cl, and (c) ± 200 ppm (EPMA) versus ± 14 ppm (SIMS) for S, respectively.

2. Comparison of analytical results of H₂O in silicic melt inclusions with SIMS and FTIR

We additionally analysed the H₂O content of six silicic (dacitic and rhyolitic) melt inclusions using a DIGILAB FTS 7000 Series Fourier transform infrared (FTIR) spectrometer at JAMSTEC. This instrument is equipped with an infrared microscope (DIGILAB UMA 600), a heated ceramic (Globar®) source, KBr beam splitter, and N₂-cooled MCT detector. The spectrometer is under N₂ gas purge to eliminate the effects of atmospheric interferences. The background and sample spectra (450–6000 cm⁻¹) were accumulated over 512 scans at a resolution of 8 cm⁻¹ and at an aperture size of 10×10 μ m. Melt inclusions were doubly-polished, and the H₂O content was quantified using the peak height of the infrared absorption band at

$\sim 3500\text{ cm}^{-1}$ due to the fundamental stretching of both molecular H_2O and structurally bound OH. We followed the analytical procedures and molar absorption coefficients for dacitic and rhyolitic glasses of Yamashita *et al.* (1997). The H_2O contents of the six silicic melt inclusions analysed with SIMS and FTIR are compared in Fig. S2. Generally, the analytical results with FTIR are higher than those with SIMS and the differences increase with increasing SiO_2 (Fig. S2), thus, we use the H_2O data analysed with FTIR for these six silicic melt inclusions.

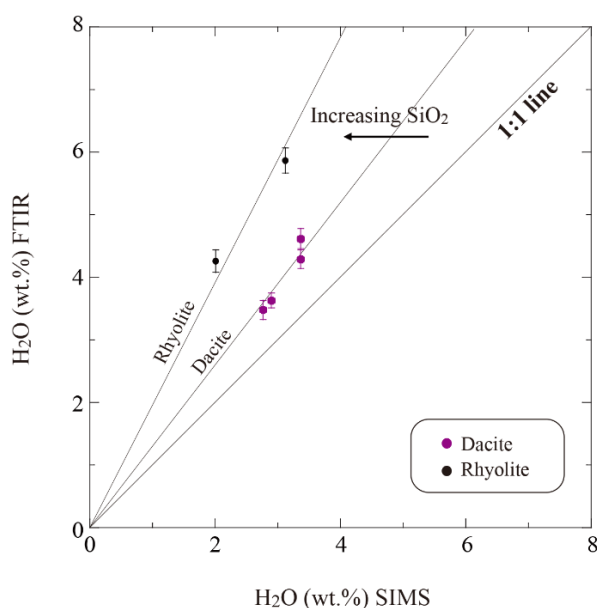


Fig. S2 Comparison of analytical results of H_2O with SIMS and FTIR. Analytical results of H_2O with SIMS are systematically lower than those results with FTIR with increasing SiO_2 in melt inclusions. The analytical uncertainty of H_2O with FTIR ($2\sigma = 0.16\text{ wt \%}$) was determined by repeated analysis of melt inclusions. Analytical uncertainty of H_2O with SIMS ($2\sigma = 100\text{ ppm}$, determined by repeated analyses of EPR-G3 reference glass; Shimizu *et al.*, 2017 & 2019) are too small to indicate in this diagram.

3. Results of K-means cluster analysis of the 237 melt inclusions

Results of the statistical analysis of the 237 melt inclusions by K-means cluster analysis (KCA), including their principal components and independent components are given in Supplementary Data Table S2. The variations in each major element in centred log-ratio (*clr*) for each cluster are graphically summarised in Fig. S3. The cluster numbers (1–5) are assigned in the order of the mean values of *clr* SiO_2 ; the mean value of *clr* SiO_2 is the lowest for Cluster

1 and is the highest for Cluster 5 (Fig. S3a). The results of KCA plotted on diagrams of *clr*-transformed oxide composition versus *clr* SiO₂ are shown in Fig. S4.

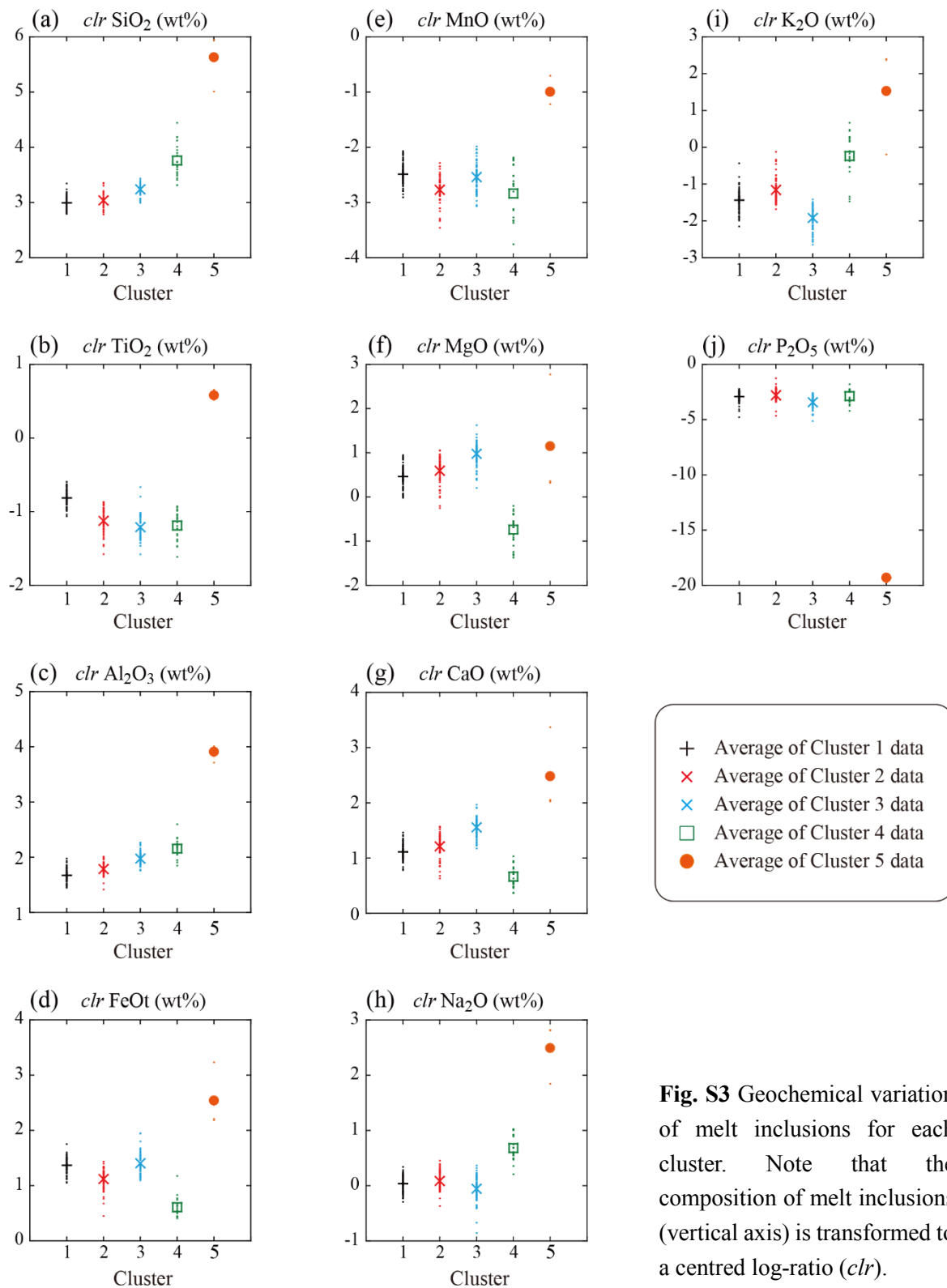


Fig. S3 Geochemical variation of melt inclusions for each cluster. Note that the composition of melt inclusions (vertical axis) is transformed to a centred log-ratio (*clr*).

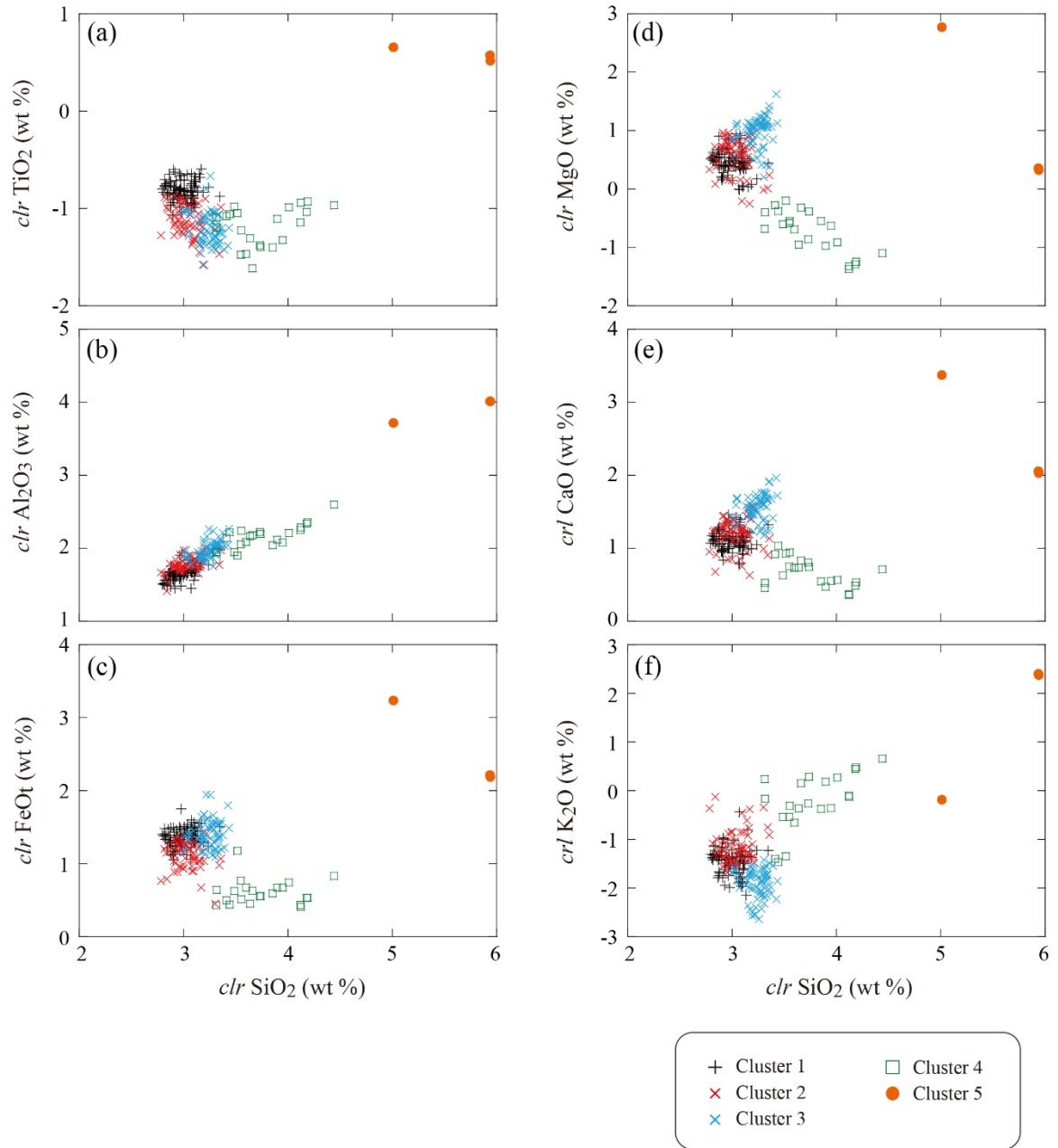


Fig. S4 The results of KCA plotted on diagrams of centred log-ratio (*clr*) transformed oxide composition versus *clr* SiO₂.

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