Processing large FORC diagram datasets applied to Earth-Science research

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Quantifying magnetic particle ensembles in rocks and sediments is a fundamental task in all paleomagnetic and environmental magnetic studies. The magnetic state of a particle is highly sensitive to its size and shape, changing from superparamagnetic (SP) to stable single domain (SD) to pseudosingle-domain (PSD) and finally to multidomain (MD) as the particle size increases from a few tens of nanometers to several tens of micrometers. Natural samples contain a complex, multicomponent mixture of different magnetic phases with a wide range of particle sizes derived from a variety of possible sources. The convolution of magnetic signals from these different mineral populations results in complex bulk magnetic signatures, which reflect the totality of factors that have influenced the history of the magnetic ensemble, e.g., crystallization or depositional conditions, weathering and alteration, provenance, transport processes, climatic and environmental variability, etc. While current techniques are successful at revealing qualitative trends in behavior, they do not lend themselves readily to obtaining an unambiguous quantitative unmixing of the SP, SD, PSD, and MD fractions present. First-order reversal curve (FORC) diagrams provide a potential solution to this problem. FORCs are highly sensitive to variations in grain size. This sensitivity derives from the strong variation in magnetic domain state with increasing grain size, which manifests itself in FORC diagrams as a gradual change from horizontal to vertical spreading of the FORC distribution. FORCs allow researchers to fingerprint domain states, extract coercivity distributions for these domain states, and detect geometry-specific magnetostatic interaction fields rather unambiguously. Here we present a magnetic component unmixing method based on principal component analysis (PCA) of FORC diagrams of natural samples. PCA provides an objective and robust statistical framework for unmixing, because it represents data variability as a linear combination of a limited number of principal components that are derived purely on the basis of natural variations contained within the dataset. For PCA we resample FORC distributions on grids that capture diagnostic signatures of magnetic domain states. Individual FORC diagrams are then recast as linear combinations of end-member (EM) FORC diagrams, located at user-defined positions in PCA space. The EM selection is guided by constraints derived from physical modeling, and is imposed by data scatter. The subjectivity of EM selection can be minimized by including constraints from granulometric filtering, physical modeling, additional datasets, or standard reference FORCs. The method works best when the sample suite covers a large region of mixing space. However, even when the variability is limited, PCA still does a reasonable job of revealing the nature of the EMs. Although initially designed with sediments in mind, the method presented here can equally be applied to rocks, meteorites, as well as to synthetic materials. The method lends itself readily to automation and can be easily incorporated into existing FORC processing packages.