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New strategies for 2D and 3D microstructural analysis: Insight on trace element diffusion in naturally deformed pyrite

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Techniques for nanoscale geochemical and structural analysis are typically rooted in the material sciences. In recent years, analytical tools including electron channelling contrast imaging (ECCI) and atom probe tomography (APT) are increasingly applied to geological materials. Whereas ECCI allows for the direct observation of crystal defects at the nanometer scale, APT can investigate the composition crystalline material by detecting individual atoms. Herein we bridge the gap between material sciences and geosciences by combining electron backscatter diffraction (EBSD), ECCI, and APT on pyrite in an attempt to better understand the underlying physicochemical processes that mobilize trace elements during plastic deformation. The combined results reveal crystal distortion and crystal-plastic deformation in the form of increased dislocation density, stacking faults, bend contours, and low-angle grain boundaries that are found decorated by elevated As and Co compositions. Trace element depletion in the wake of dislocations' displacement direction and the absence of a chemical potential gradient support a dislocation-impurity pair (DIP) diffusion model. However, we also document evidence that multiple diffusion mechanisms such as pipe and volume diffusion may have acted simultaneously. In addition, we applied a new data processing technique that allows for orientation measurement of nanostructural crystal defects detected by APT. Dislocations within our investigated sample plot along 110 planes suggesting slip on (110). Since the entrainment of trace elements into migrating dislocations can decrease their velocity and cause stress serrations, we can assume that DIP diffusion could potentially lead to premature strain hardening and play a significant role in a mineral's deformational behaviour. Further investigation on DIP diffusion using these innovative strategies could lead to a better understanding of the rheology of minerals and materials, and could have a significant impact in the fields of geosciences and material sciences.