

On twinning and microstructures in calcite and dolomite

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ABSTRACT

Apparent superlattice reflections obtained in electron diffraction patterns of modulated calcite and dolomite have been ascribed to local domains of various different metastable Ca-Mg ordering schemes that are not known as macroscopic phases. We show that the type “c” reflections in diffraction patterns of supposed superstructures can in fact be produced by superposition of diffraction from the host crystal and that from domains that are in an orientation related to the host by twinning on (104). From details of the additional reflections present, we deduce that the carbonate anions are orientationally disordered in the twin nanodomains, which have the $R\bar{3}m$ space group of high-temperature disordered calcite. This twinning can explain the diffraction ascribed to type “ γ ” μ ” ν ” superstructures, and resolves controversies over the occurrence of these purportedly different superstructures. The relationships between composition, orientational order of the carbonates, molar volume and known macroscopic structures, and the possibility of interfacial strain reduction by static disorder in the twin domain, are discussed. We stress the importance of checking for presence of twinned nanodomains using microdiffraction before attributing an apparent superstructure modulation to local cation ordering. High-resolution imaging may not be diagnostic, since overlap of small domains and host matrix can give Moiré patterns that resemble superlattice fringes.

Keywords: Calcite, dolomite, twinning, superstructures, electron diffraction