Coexistence of twisted and untwisted crystals: An impurity/structural order model with implications for agate patterns

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ABSTRACT

Coexistence of twisted and untwisted crystals is explained via a model that accounts for the coupling of the entropic and energetic effects of impurities and a supra-lattice-scale structural order parameter. It is shown that twisted impure crystals can be in equilibrium with untwisted purer ones. The model explains how coexistence can occur in agates and other systems under hydrostatic stress. The model implies that untwisted crystals grown under one set of conditions could undergo a phase separation that, when accompanied by an imposed compositional gradient, leads to commonly observed, alternating bands of twisted and untwisted crystals and, when occurring in the absence of an external gradient, mossy patterns of crystal texture can emerge. This phenomenon is not related to anisotropic applied stress. Rather coexistence is a consequence of a compositional segregation/twist phase transition. Since twist coexistence is a compositional equilibrium, it arises from the exchange between bulk phases; hence, the detailed nature of the atomic structure within an interface between twisted and untwisted zones is not relevant. The approach places crystal-twist phenomena within the theory of order/disorder phase transitions.

Keywords: Agate, agate banding, free energy model, phase separation, quartz fibers, self-organization, twisted crystals, twisted/untwisted crystal equilibria

INTRODUCTION

Crystals that exhibit a twisted habit have long been recognized and many examples have been described in a variety of minerals (Frondel 1936; Spencer 1921). In large crystals, progressive changes in orientation of the crystal lattice are represented by obvious curvature of crystal faces and may result in a pronounced helical twisting of elongated crystals (Frondel 1936; Spencer 1921). In small crystallites or fibers, twisting is generally not obvious upon megascopic examination, but is easily identified by the sweeping extinction in thin section when viewed with polarized light under crossed polars (Frondel 1978; Milliken 1979) (Fig. 1). Sweeping extinction documents the changing orientation of a crystal lattice along the length of the fibers.

While the phenomenon of twisting has long been known, the causes are less well understood. Explanations for crystal twisting include twinning (Kozlova and Belov 1981; Xu et al. 1998), point and edge defects (Radke and Mathis 1980; Searl 1989), lattice dislocations (Frondel 1978; White and Wilson 1978), and ionic substitutions and interstitial defects (Heaney and Davis 1995; Wang and Merino 1990).

Spencer (1921) stated that twinning is a common cause of twisted crystal habits. Kozlova and Belov (1981) concluded that Brazil twinning accounted for curved prism faces in α-quartz, and observed that the intergrowth of twinned crystals produces a fine mosaic structure that imparts an apparently continuous curvature to prism faces. Xu et al. (1998) showed that Brazil twinning accounted for most of the atomic-scale defects in fibrous chalcedony, and a high density of twin boundaries, sometimes forming discrete domains of the silica polymorph moganite, has been documented at the unit-cell scale (Heaney and Davis 1995; Xu et al. 1998). Zebraic chalcedony (Fig. 1) is a classic example of twisting of crystalline fibers along the axis of elongation (Milliken 1979).

Saddle structure in dolomite has been explained as due to curvature caused by substitution of Ca for Mg or the introduction of extra Ca-depleted layers as edge defects in the dolomite lattice (Barber et al. 1985; Radke and Mathis 1980; Searl 1989). Following this notion, Wang and Merino (1990) attributed twisting of chalcedony fibers in agate to the substitution of Al for Si in tetrahedral lattice sites. Heaney and Davis (1995) confirmed the coupled substitution of Al3+ and Na+ for Si4+ in agate chalcedony using secondary ion mass spectrometry.

Twisting of crystals during periods of deformational strain is also well known (Williams and Urai 1989), and curved fibers have been used to quantify the strain associated with different deformational phases (Carminati 2001; Durney and Ramsay 1973). Crystal fibers may twist as they grow in response to syntectonic deformation (Durney and Ramsay 1973) or they may bend during subsequent deformational strain (Williams and Urai 1989) or both (White and Wilson 1978). The twisting is caused by multiple lattice defects that include voids (bubbles), lattice

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