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Epitaxial Growth of Gypsum on Anhydrite: In situ AFM Observations and Computer Calculations

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The transformation of anhydrite ($CaSO_4$) into gypsum ($CaSO_4$ $2H_2O$) is a common phenomenon in many gypsum deposits. It seems that the gypsification process occurs preferentially on anhydrite cleavage surfaces and pseudomorphic replacements have been frequently observed (Warden and Pallister, 1968) [1]. However, the formation of secondary gypsum from anhydrite is not yet well understood and some possible alternative mechanisms have been proposed: dissolution-precipitation, direct hydration of anhydrite surfaces or stepwise hydration via bassanite (Holliday, 1970). In addition, the similarities between gypsum and anhydrite structures suggest the possibility of development of epitaxial and topotaxial phenomena. Epitaxial growth of gypsum on anhydrite can be considered as indicative of a subsequent transformation.

In order to obtain some information about the surface processes which relates gypsum and anhydrite, we have conducted a number of *in situ* Atomic Force Microscopy (AFM) experiments at room temperature. By passing Ca-SO_4 concentrated aqueous solutions (10 - 70 mmol/l) over anhydrite (100) cleavage faces, the epitaxial growth of gypsum monolayers can be promoted. AFM observations show that the deposition of gypsum on anhydrite is highly anisotropic and proceeds by alternating layers with reversed high growth rate directions ($R_{<001>}$ ~12 nm/s). Moreover, the advancement of gypsum layers is strongly controlled by the anhydrite substrate. Typically, a monomolecular gypsum layer starts to grow from pre-existent anhydrite cleavage steps (usually parallel to <011> directions and ~ 7 Å in height) and it advances until a higher anhydrite step edge is reached. Then, a new gypsum monolayer grows in the opposite direction on top of the previous one. Two layers of gypsum seem to have the same height as one anhydrite cleavage step and no discontinuities on the surface are observed after growth. Goniometric measurements indicate that the main epitaxial relationships are: $(100)_{anhydrite}//(010)_{gypsum}$ and $[001]_{anhydrite}//[001]_{gypsum}$. The gypsum-anhydrite epitaxial relationships observed during the AFM experiments can be explained on the basis of structural similarities and interaction energies between both surfaces. Molecular simulations were carried out using the Cerius[2] and GULP computer programs. We modelled an anhydrite (100) - gypsum (010) interface by considering different orientations of a rhombohedral-shaped gypsum cluster bounded by [100] and [001] edge directions. Since water molecules seem to play an important role in the development of the epitaxy, calculations have been made assuming that one or two H_2O layers constitute the interface between anhydrite and gypsum. The lowest interaction energies calculated corresponded to the gypsum-anhydrite orientation experimentally determined.

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Holliday DW, *J. Sed. Petr*., **40**, 734-744, (1970).