ORIENTED OVERGROWTH OF BRUSHITE ($CaHPO_4 \cdot 2H_2O$) ON GYPSUM ($CaSO_4 \cdot 2H_2O$)

A.J. PINTO, A. JIMÉNEZ Y M. PRIETO

Dpto. de Geología. Universidad de Oviedo. C/ Jesús Arias de Velasco, s/n. 33005 Oviedo.

Interaction between aqueous solutions containing dissolved P (V) and gypsum results in surface precipitation of brushite ($CaHPO_4 \cdot 2H_2O$) crystals. The crystals grow oriented onto gypsum's surface, forming an epitaxy. Experiments have been carried out at 25°C and 1 atm. The prevailing aqueous species within the range of pH (from 6 to 4.6) approached by this study are $H_2PO_4^-$ and HPO_4^{2-}. The obtained morphologies of brushite consist of thin crystals elongated in the [101] direction with {010}, {1$\bar{1}$1} and {$\bar{1}\bar{1}$1} as major forms. Using an *A*-centred unit-cell setting for both brushite (*Aa*) and gypsum (*A2/a*) (Heijnen y Hartman, 1991), the epitaxy can be described by considering the matching along the common [001] and [100] directions. The mismatch, in our case, can be calculated using the following expression:

$$\text{Mismatch (\%)} = \frac{[u,v,w]_o - [u,v,w]_s}{[u,v,w]_o} \times 100$$

where [*u,v,w*] is the repeating period along the matching directions of the substrate (s) and the overgrowth (o). The obtained misfits for [001], [100] and [101] directions were of 1.3%, 2.3 % and 4.3% respectively. The unit-cell of brushite is "contracted" along [101] when compared with gypsum's, and the β angle results to be larger for brushite, with an angular misfit of 4.4 angular degrees. The brushite overgrowth forms thin platelets elongated on [101], which corresponds to the direction of the strongest PBC within its structure. Moreover, the gathered observations point towards a bi-dimensional reticular control with [001] and [100] as correspondent directions. Thus, using an A-centred unit cell setting for both minerals, the observed epitaxial relationship is $(010)_{Gy}||(010)_{Br}$, $[001]_{Gy}||[001]_{Br}$ and $[100]_{Gy}||[100]_{Br}$. The performed SEM observations point towards a mechanism of epitaxial growth with features from both *Stransky-Krastanov* and *Volmer-Weber* mechanisms (Chernov, 2003). Nanoscale studies will be made in the future in order to sort this question out.

In the present work, both crystal morphology and epitaxial orientation are approached on the basis of the bond arrangement within the structure of both minerals.

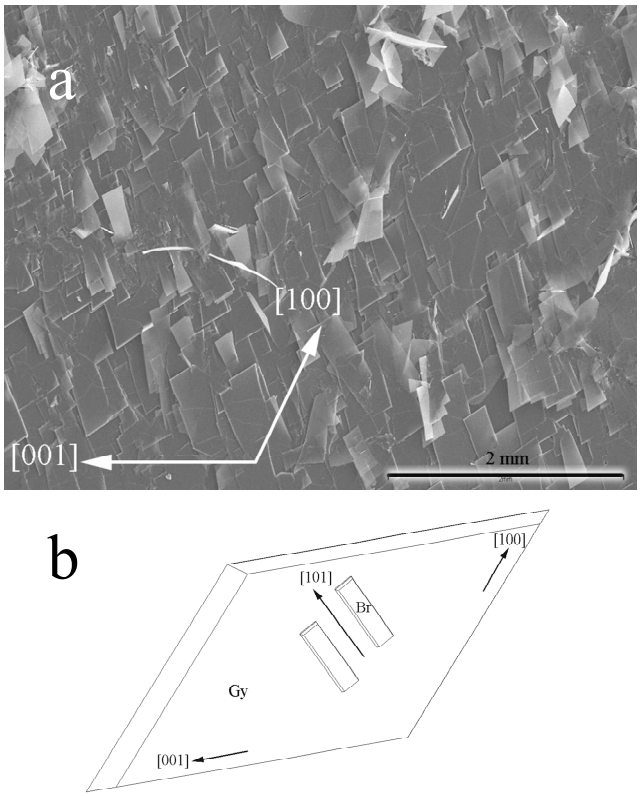

Figure 1. a) SEM image of thin brushite crystals oriented onto gypsum's (010) face, along [101]. b) Epitaxial relationships between gypsum (Gy) and brushite (Br). An A-centred unit-cell setting was used for both minerals.

REFERENCES

Heijnen, W.M.M. y Hartman, P. (1991). J. Cryst. Gr., 108, 290-300.

Chernov, A.A. (2003). Modern Crystallography III. Crystal Growth. Springer-Verlag, Berlin.