Piezoelastic Constants of Retgersite (NiSO4·6H2O)

Arbeck, Dirk[1] Haussühl, Eiken[1] Bayarjargal, Lkhamsuren[1] Paulsen, Natalia[1]
[1]Goethe-Universität Frankfurt am Main, Inst. für Geowissenschaften, Altenhöferallee 1, 60438 Frankfurt am Main

The crystal structure of retgersite ($NiSO_4 \cdot 6H_2O$) was determined by Beevers and Lipson (1932) who were, however, unable to locate the positions of the hydrogen atoms. Later refinements were published by O'Connor and Dale (1966) and Stadnicka, Glazer and Koralewski (1987). Retgersite crystallizes in space group $P4_12_12$ with a=b=6.790(3) Å and c=18.305(4) Å. The elastic stiffness coefficients and the four thermoelastic constants were measured by Stoianoff and Missell (1982) in the temperature range of 4 – 300 K. However, the piezoelastic constants have not yet been investigated. In the present study, large single crystals of $NiSO_4 \cdot 6H_2O$ were grown from aqueous solution. The elastic stiffness coefficients and the piezoelastic constants of synthetic $NiSO_4 \cdot 6H_2O$ were then determined experimentally in a pressure range from 1 to 500 bar using ultrasonic resonance techniques at room temperature (298 K) combined with a gas-loaded autoclave.

For P=1 bar, the elastic stiffness coefficients (not corrected with respect to the piezoelectric effect) are (in GPa): c_{11}= 46.1(5), c_{33}= 34.6(4), c_{44}= 10.9(5), c_{66}= 21(1), c_{12}= 38(1) and c_{13}= 25.4(8). These values agree within 6 % for c_{11}, c_{33}, c_{44}, c_{66} and c_{12} with the data published earlier by Stoianoff and Missell (1982). However the agreement for the transverse coefficient c_{13} is only within 20 %. The reason for this is still unknown and is the subject of further investigations. The piezoelastic constants of the longitudinal and shear modes at 500 bar are: p_{11}=4.8(5), p_{33}=7.0(7), and p_{44}=1.6(2), p_{66}=3.0(3), respectively.

In this study, a detailed comparison of the thermoelastic and piezoelastic constants will be given. Furthermore, the anisotropic behaviour of the longitudinal elastic stiffness and of the piezoelastic stiffness will be interpreted with respect to the crystal structure, in particular to the hydrogen bonding system.

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