Employing Polyethylene as Contacting Agent Between ATR-crystals and Solid Samples with Hard Surfaces

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Modern attenuated total reflection (ATR)-spectroscopy appeared at the end of the 5th decade and the beginning of the 6th decade of the previous century. Since then it has found widespread use for the structural investigation especially of liquids and soft solids like polymers etc. For samples with hard surfaces, e.g. most of the inorganic single crystals, ATR-spectroscopy has a shadowy existence due to the need of establishing an intimate contact between the incidence medium (i.e. the ATR-crystal) and the medium under investigation.

All proper techniques presented so far, however, show either the disadvantage of being comparably complicated to use or of employing toxic and volatile liquids. The aim of this work is therefore to introduce a technique that is easy to apply and assures optical contact using a non-toxic and easily removable coupling agent.

To assess the quality of polyethylene as contacting agent we conducted IR-ATR experiments employing an ATR-ZnSe semi-sphere as ATR-crystal and an optically polished (001)-cut of a fresnoite (Ba_2TiSiO_8, optically uniaxial) single crystal. Both s- and p-polarized infrared spectra were recorded at different angles of incidence ranging from 10° to 80°. These spectra were compared with a second series of spectra where we employed CS_2 as immersion liquid, which is the reference material known from literature [1], and with artificial spectra modelled from previously obtained single crystal data [2]. Since the employment of polyethylene results in a superior resemblance between measured and modelled spectra and is much easier and safer to apply, we expect this technique to open up the way for a routine application of IR-ATR spectroscopy to materials with hard surfaces.

[1] G. Kortüm, Reflectance Spectroscopy: Principles, Methods, Applications, Springer-Verlag, Berlin-Heidelberg-New York, 1969.

[2] T.G. Mayerhöfer, H.H. Dunken, Vibrat. Spectr. 25 (2001) 185.