UV-VIS reflective spectroscopy measurement of optical functions and of certain energy characteristics specific to sulphurous minerals (Sphalerite, Galena, Chalcopyrite)

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The paper aims at determining the energetic and structural properties of sulphurous minerals such as sphalerite, galena and chalcopyrite found in the mining region of Maramures, Romania, through UV-VIS optical reflectance spectrophotometric measurements.
The energy states of minerals depend on the placement of composing atoms and also on the evaluation of energy states of the electrons within the composing atoms which permits a better understanding of the differences between ideal and real (with structural defects) crystals that exist in nature.
The spectrophotometric measurements were taken in the 200-900 nm range, the reflection spectrum obtained being processed based on the Krames-Kronig formalism which allowed us to determine the optical functions of these minerals.
These functions were: The optical adsorption coefficient, the refraction index, the effective valence number, the real and imaginary part of the dielectric constant (reveals information about the interaction mechanism between light and electrical charge bearers), the characteristic loss functions of the electrons (give information about the spectral evolution of the energy states).
The first two coefficients allow us to determine the penetration depth of the beam in the interaction medium allowing the optimization of the evaluations through optical reflection spectrophotometry.
The special van Hove points were highlighted and the Argand diagrams were drawn, that allowed us to determine the base exciton bands domains for the minerals in question.
The van Hove inflection points permit the estimation of the minimal energy interval between the valence Band (VB) and the conduction band (CB) for the sulphurous minerals in discussion.
There were obtained, for galena, the value of the interdicted pseudo-band of about 0.43 eV, for sphalerite 1.5 eV and for chalcopyrite 1.42 eV, for the energy areas close to the van Hove inflexion points.
The results obtained (optical functions and energy parameters determined directly through the Kramers-Kronig model) allow us to optimize the use of optical reflection spectrophotometric methods in the study of sulphurous minerals taking into account the compositional and structural variety of these which leads to particular properties function of the nature of the mineral and also of its geological source.

References:
Todoran R., Sharkany J. (1998), Journal of Mining and Metallurgy, vol. 34 issue 1-2, 57-65.
L. van Hove (1953), Phys. Rev. 89, 1189.
Olli Haavisto (2009), Reflectance Spectrum Analysis of Mineral Flotation Froths and Slurries, Yliopistopaino, Helsinki, 16.
Querry, Marvin (1987), Optical Constants of Minerals and Other Materials from the Millimeter to the Ultraviolet, 153-158.