Identification of substances from diffuse reflectance spectra of a broadband quantum cascade laser using Kramers-Kronig relations

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Abstract. A real-time automated system for remote substance identification on various surfaces without preliminary sample preparation is presented. In practice, it can be used, for example, as an alerting system to signal the presence of some contaminants. The main components of the system are diffuse reflectance spectra acquisition module, data processing module, and identification module. Development of each module was based on the choice of appropriate devices and algorithms, either existing or newly designed. The experimental setup consists of a quantum cascade laser emitting in the spectral range of 5.3 to 12.8 pm with a HgCdTe photodetector. To achieve better selectivity of substance recognition, identification algorithms were based on the absorption and transmission spectra calculated from the recorded diffuse reflectance spectra. Spectra conversion algorithms employed Kramers-Kronig relations, phase spectra extrapolation, and phase correction. The system was supplied with the recognition database composed of certain commercially available substances. The experiments showed that the usage of transmittance spectra significantly improved the sensitivity of the identification method; the remote identification limit of 30 pg acetylsalicylic acid has been experimentally confirmed. For similar substances, such limit was estimated as 10 pg /cm2 at a distance of 1 m.

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