Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Elimination of Optical Artifacts from Transmission FTIR Spectra for Quantitative Bond Density Analysis MILAN MILOSEVIC, MeV Technologies, SEAN KING, Intel Corporation — Fourier transform infrared (FTIR) spectroscopy is a powerful technique for characterizing the chemical structure and the short range order in bulk solids and thin films. However, transmission FTIR spectra of thin films deposited on optically thick substrates are complicated by the presence of numerous "optical effects" that arise from reflections at the two surfaces and the interface of the film and substrate. The convolution of these "optical effects" with the true absorption spectrum of the film can cause quantitative analyses of FTIR spectra of the films on substrate to yield errors as large as 90% in integrated absorbance and other quantitative parameters. In this report, we describe and demonstrate a method that enables such "optical effects" to be removed with complete rigor allowing the true absorption coefficient spectrum of the film to be obtained. Unlike prior methods that address the problem as a combination of coherent and incoherent reflections in the film and substrate respectively, we use the exact theoretical expression for the transmittance of a thin film on an optically thick substrate. We show that this allows us to naturally separate the undesired "optical effects" and desired thin film absorption spectrum into two separate terms. Using both simulated and experimental data we demonstrate that the term containing "optical effects" can be cleanly subtracted from the experimental FTIR spectra to yield the true absorption coefficient spectrum of the thin film allowing for rigorous quantitative bond density and, potentially, elemental composition of the films to be calculated from the thus corrected spectra.

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Date submitted: 15 Nov 2013 Electronic form version 1.4