

FINITE-DIFFERENCE TIME-DOMAIN MODELING OF FREE INDUCTION DECAY SIGNAL IN CHIRPED PULSE MILLIMETER WAVE SPECTROSCOPY

ALEXANDER HEIFETZ, SASAN BAKHTIARI, HUAL-TEH CHIEN, *Nuclear Engineering Division, Argonne National Laboratory, Argonne, IL, USA*; KIRILL PROZUMENT, *Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL, USA*; STEPHEN K GRAY, *Nanoscience and Technology Division, Argonne National Laboratory, Argonne, IL, USA*; RICHARD M WILLIAMS, *Detection Systems, Pacific Northwest National Laboratory, Richland, WA, USA*.

We have developed computational electrodynamics model of free induction decay (FID) signal in chirped pulse millimeter wave (CPMMW) spectroscopy. The computational model is based on finite-difference time-domain (FDTD) solution of Maxwell's equations in 1-D. Molecular medium is represented by two-level system derived using density matrix (DM) formulation. Each cell in the grid is assigned an independent set of DM equations, and thus acts as an independent source of induced polarization. Computer simulations with our 1-D model have shown that FID signal is propagating entirely in the forward direction. Intensity of FID radiation increases linearly along the cell length. These results can be explained analytically by considering phases of electromagnetic field radiated by each independent region of induced polarization. We show that there is constructive interference in the forward in forward direction, and destructive interference in backscattering direction. Results in this study are consistent with experimental observations that FID has been measured in the forward scattering direction, but not in backscattering direction.