CONVOLUTION PROBLEMS IN TIME-RESOLVED X-RAY DIFFRACTION

S. Bratos, J.-Cl. Leicknam

Laboratoire de Physique Théorique
de la Matiére Condensée,
Université Pierre et Marie Curie, Case courrier 121
(*4, Place Jussieu, Paris 75252, Cedex 05, France*)

S u m m a r y

Convolution problems in the time-resolved scattering of 10–1000-ps x-ray pulses are studied theoretically. The model system is a diluted solution of diatomic molecules A_2 dissolved in an inert solvent. This system is submitted to a sub-picosecond laser pulse, which promotes the molecules A_2 into an excited electronic state. The molecule then return into their ground state, passing through several intermediate electronic states. The effects of the finite duration of probing x-ray pulses on various x-ray signals are then examined in the frame of this model. Unbiased signals generated by very short x-ray pulses are explored first. Variations of a molecular geometry during this process are clearly visible in r-resolved, but are less explicit in q-resolved signals. The signals measured with x-ray pulses of a finite duration are studied next. Atomic motions remain detectable, but only if the x-ray pulses are shorter than or comparable to the times of a molecular dynamics. Here again, the r-resolved signals are more appropriate for monitoring the molecular dynamics than q-resolved signals. Finally, the effect of the insufficient temporal location of probing x-ray pulses with respect to that of exciting laser pulses is examined. It is shown that this last effect can be accounted for by simply replacing the true x-ray pulse intensity by another theoretically predicted intensity. The similarity of deconvolution techniques in spectroscopy and in time-resolved x-ray diffraction is strongly emphasized.