

CHAPTER 5

CONCLUSION

ATR spectral intensity is directly related to quantitative characteristic of the material. However, in order to extract quantitative characteristic or gain an insight understanding about the system being investigated, several parameters have to be verified. All equations concerning ATR spectral intensity assumed optical contact between IRE and sample. Thus, it is necessary to verify optical contact in the system before further analyze spectra. In most laboratories, multiple reflection ATR (MATR) accessory is available instead of a single reflection accessory. An effective number of reflections must be verified in order to utilize the observed spectra for quantitative analysis purpose.

The proposed technique for calculating number of reflections in an IRE enables one to calculate the effective number of reflections in an IRE of an MATR accessory by using experimental results. The calculated value is always smaller than the theoretical value. This is due to beam divergence and accessory alignment. In order to obtain a reliable result, an isolated peak with a small absorption and good signal-to-noise ratio must be employed for the calculation.

The optical contact between solid sample and the IRE can be improved by thin organic film. The contact is improved even when the organic film is disappeared. ATR spectral intensity of solid sample is greatly enhanced. The enhancement is greater in case of a glassy polymer (PC sample) than a rubbery polymer (PVC sample). This is because PVC itself has a good contact with the IRE, the air gap is rarely exist. The spectral intensity of ZnSe/*i*-propanol/PC system is increased the most since PC sample alone rarely has optical contact with the IRE. Evaporation of *i*-propanol induces capillary force to adhere PC sample to the IRE.

However, from the experimental result, it was found that an optical contact still cannot be obtained perfectly.

The proposed equation for the determination of the sampling depth agrees quite well with the experimental results and also with the simulated data. The sampling depth varies with wavenumber and spectral intensity. The sampling depth calculated at high wavenumber can be experimentally verified by comparing with the thickness of liquid film at which its spectral intensity decreases significantly from its bulk intensity (i.e., same order with the noise level).