Model of the Electromagnetic Contribution to Wurface Enhanced Raman Scattering (SERS)

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In this work, we present a theoretical model of the electromagnetic contribution to surface enhanced Raman scattering (SERS). The SERS effect is characterized by the enormous intensification of the Raman emission of molecules, when these are adsorbed on a metallic surface (with nanometric roughness). This intensification is several orders of magnitude higher than the Raman emission of isolated molecules. In recent years, SERS spectroscopy has improved in sensitivity so as to make possible the detection of a single molecule on a nanostructured substrate [1]. The SERS effect is due to the combined action of chemical and electromagnetic enhancement mechanisms. Leaving aside the contribution of the chemical mechanism, this is possible provided that there is a huge concentration of electromagnetic field on certain points of the substrate, due to the excitation and localization of surface plasmons [2–4].

We thus investigate the electromagnetic mechanism that is responsible for such surface-plasmonind-uced, electromagnetic field enhancements. Our theoretical model incorporates the Raman response of a metallic surface covered with a dipole layer. The calculation of the scattered electromagnetic field is based on the exact Green's theorem integral equation formulation. With this model we are able to calculate the surface field, near field, and far field at the Raman-shifted frequency, separately of the electromagnetic field at pump frequency. A rigorous calculation of the scattered electromagnetic field has been carried out for random metal surfaces with similar properties to those exhibited by nanostructured metal substrates used in SERS. Numerical results are presented for single realizations, along with mean values of the SERS enhancement factor averaged over an ensemble of realizations [1].

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