Determination of Multilayer Structures from Grazing Incidence X-Ray Reflectometry Measurements Using a Simulated Annealing Algorithm

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Grazing incidence x-ray reflectometry (GIXR) using middle x-rays ($\lambda \sim 0.15$ nm) is a characterization technique routinely available at laboratories involved in the manufacturing of thin films and nanometer-scale multilayers. The technique is particularly useful during the calibration phase when a series of samples are made to define the relation between the material growth conditions and the multilayer parameters, namely the thickness, density, and interface roughness of the layers. The method has also been used in-situ to monitor the performance during growth.[1] In absence of a feedback control system during multilayer growth it has often been observed that the time between a calibration run and the next deposition run should be as short as possible. Therefore, fast GIXR data acquisition and analysis are required.

We report here on our attempt to automatize the GIXR data refinement procedure, which is normally very time-consuming and needs much expertise. The reflectometry data was fitted to a model based on the x-ray dynamical theory. Each layer was described by its chemical composition, thickness, density, and rms roughness interface of width σ (Gaussian interface profile).[2] We have used a probabilistic optimization algorithm, known as simulated annealing (SA) algorithm,[3] which is well suited to problems containing a high number of parameters. In principle, the routine is able to find the global minimum of a given cost function, here the distance between the calculated and the experimental data points, independent of the choice of the initial guess. A control parameter, noted temperature, is first set to allow many solutions to be tested. When slowly decreased, it progressively reduces the field of possibilities to the nearest neighbors. A series of solutions are evaluated for each temperature and are assigned a probability depending on the magnitude of the cost function (Metropolis algorithm). The number of iterations must be large enough to simulate a thermodynamical equilibrium.

To find the SA model that best suits our particular problem we have studied the influence of several cost functions on the final parameters as well as various ways of searching for neighbors and of decreasing the temperature. The results will be illustrated by the analysis of a Ni/B_4C sample for which 120 parameters were evaluated. The initial guess and the background noise level were found to critically influence the final solution. Compensations between variables have been observed but could be identified based on materials growth information.

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