Optimization of a simulated annealing algorithm for the design and characterization of x-ray multilayers.

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A x-ray multilayer is either described by its geometrical parameters (chemical composition, thickness, density, interface roughness) or by its x-ray response (energy or angular spectrum of reflection or transmission). Although the prediction of the x-ray performance from a set of multilayer parameters is in principle straightforward, the reverse case, known as inverse problem, is far more difficult to solve. Unfortunately, the latter one is more often encountered: at the design level, when one must find a multilayer sequence capable of generating a given spectrum, and during the production phase when one must calibrate the layering process from the x-ray response of test samples.

To cope with the large number of parameters involved, we have implemented a Markovian probabilistic optimization algorithm, known as simulated annealing (SA). Various merit functions and ways of varying the annealing temperature parameter have been investigated to match the specific case of multilayers described by their x-ray diffraction properties. The Cauchy and Gauss distributions turned out to best select the neighbor solutions. However, although the principle of the Metropolis algorithm suggests that a global solution is always to be found, experience shows that, in certain cases, unmanageably large execution times are required to find this solution. The initial guess was found to critically influence the convergence speed. Compensations between variables (e.g. thickness and density) have been observed which result into the presence of multiple solutions. A deficit in experimental data may be responsible for this situation. However, such a dilemma can be eluded when the growth process is well under control. For the SA algorithm to efficiently infer the multilayer parameters from a x-ray spectrum, it is necessary to provide a pre-estimation of the solution. We have chosen the Fourier analysis of the x-ray spectrum, as proposed by Bridou et al.[1] and Voorma et al.,[2] to get an estimate of the mean roughness and thickness parameters. In the case of quasi-periodic multilayers, these estimated values, used as guess to start the SA algorithm, turned out to be adequate to successfully solve the inverse problem. Means of improving the speed of convergence are now under study.

1 F. Bridou and B. Pardo, SPIE Proc. vol. 2253, p. 667-78 (1994).

2 H. J. Voorma, E.Louis, N. B. Koster, F. Bijkerk, and E. Spiller, J. Appl. Phys. **81,** 6112-9 (1997).