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Genetic algorithms used in model finding and fitting for neutron reflection experiments

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Abstract

A fitting procedure based on genetic algorithms is described. This procedure is used to find scattering length density profiles that correspond to measured neutron reflectivity data. It gives parameters of a model that fits the data, without any a priori knowledge about the sample. It can give different parameter sets of a model, that yield equally good fits to the data, which stresses the nonuniqueness of the solutions.

1. Introduction

Genetic algorithms have been studied for over 30 years. They are applied to many fields, ranging from designing jet-turbines to model fitting of seismic data [1]. It is based on the hypothesis of evolution of a species by survival of the fittest individuals within a population. The individuals can create offspring by sexual reproduction. The keyword "sexual" points to the fact that information which makes an individual fit enough to survive and hence to reproduce is combined with information of an other individual. The resulting offspring can be even more fit. This mixture of information induces a higher rate of evolution of a population than simple reproduction and an occasional mutation. The way this is done in nature is by means of genes and chromosomes. The trick of genetic algorithms is to create a "genetic code" that describes the model, and can be manipulated as natural genes. This is described in the next section. More about the ideas behind genetic algorithms can be found in Refs. [2, 3].

2. Fitting procedure

When a genetic algorithm is applied to model fitting, the genetic code consists of a bit stream. Every parameter of a model is discretized into a number of bits between an upper and lower limit. All these binary parameters are put in a fixed sequence in a one-dimensional array to construct a bit stream. With this genetic code manipulations of sexual reproduction and mutation can easily be done by manipulating bits. Sexual reproduction is simulated by taking two bit streams, cutting them at the same random position and swapping two counter parts to create two new bit streams. Mutation is simulated by occasionally changing a bit from 0 to 1 or from 1 to 0. The chance a mutation occurs can be varied and is typical 1% per bit. The fitness of a bit stream is calculated by transformation of the discretized parameters to corresponding physical parameters and calculation of the

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weighted mean squared deviation of a model from a measurement, χ^2. A pool of bit streams is created to simulate a population. Typically a pool contains between 25 and 100 bit streams. For all models in this pool (represented by the bit streams) the fitness is calculated. The next "generation" is created by mutation, sexual reproduction and survival of the fittest models. The fittest models "mate" with other fit models creating new offspring (2 models per mating) keeping the total number of models in the pool constant. Therefore half of the old-pool models are deleted. One iteration contains a calculation of the fitnesses and the creation of a new pool generation. A typical fit contains approximately 25 to 100 iterations. The initial pool is generated taking random values for the parameters.

3. Results

3.1. With a priori knowledge

The genetic algorithm was applied to measurements on reflectometer EROS of Laboratoire Leon Brillouin in Saclay [4]. A sample of 5 bi-layers of Co/Ti on a glass substrate was measured. The expected scattering length density profile as a function of z, the distance perpendicular to the surface, $\Gamma(z)$ defined by $4\pi Nb$, where N is the number density and b the scattering length of the material, is shown in Fig. 1. The measured reflectivity, $R(q)$, with q the perpendicular component of the incoming wave vector, is shown as error bars in Fig. 2. The q-resolution, Γ of substrate, Co and Ti, thicknesses, t of the Co and Ti layers and interfacial roughness, σ, were fitted. These parameters were discretized and put one after another in a bit stream. The pool contained 25 bit streams, 70 bits long, and 50 iterations were performed. A VAX-station 3100 M76 used approximately 30 min. CPU time for the double precision calculations. Relative to the time needed for the determination of the 25×50 χ^2's, virtually no time was needed for the evaluation of the genetic algorithm. After 50 iterations the best model in the pool, shown in Fig. 1, gave $\chi^2 = 3.4$. The corresponding reflectivity is shown in Fig. 2. This result was used as an initial model for a least-squares fitting procedure resulting

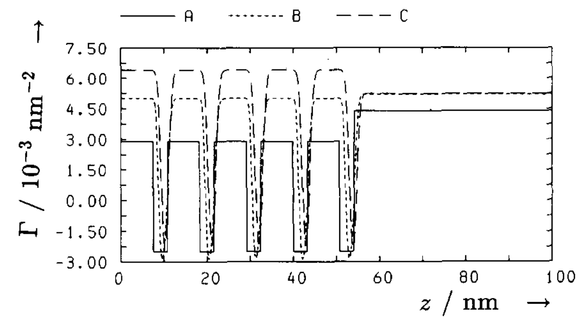

Fig. 1. Scattering length density profiles. A: model "as made"; B: best model after 50 iterations of genetic algorithms; C: model after least-squares fit.

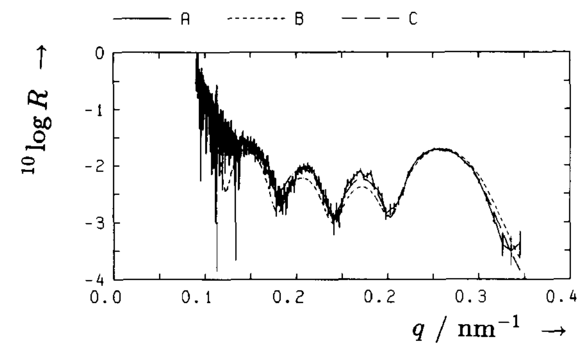

Fig. 2. Reflectivity as a function of vertical component of the incoming wave vector. A: measurement; B: best fit after 50 iterations of genetic algorithms; C: least-squares fit with initial model found by genetic algorithms.

in the model shown in Figs. 1 and 2 with $\chi^2 = 1.4$, which is satisfactory. At each interface, σ was fitted to be approximately 1 nm. Because Γ for the Ti layer ($-5.8(5) \times 10^{-3}$ nm^{-2}) did not match Γ of Ti (-2.4×10^{-3} nm^{-2}), the 24 other models in the pool were also used as initial model for a least-squares fit. For the Co layer all fits gave approximately the same Γ and t. For the Ti layer however, different combinations of Γ and t were found, resulting in fits all with $\chi^2 = 1.4(1)$. From the fact that these combinations are points on a straight line, it was concluded that a fit would also be possible for a fixed Γ of the Ti layer of -2.4×10^{-3} nm^{-2}, with $t \approx 2$ nm. Taking these values as initial conditions for a least-squares fit resulted in

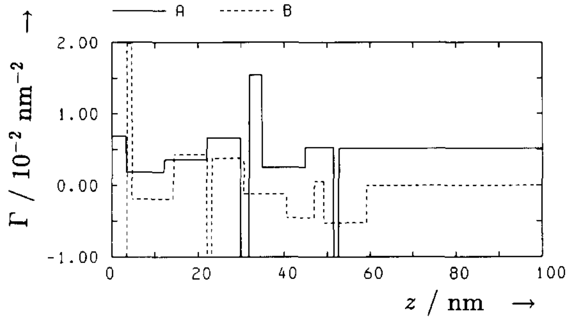

Fig. 3. Scattering length density profiles. A and B are two models which fitted the data with a χ^2 of 1.2 and 0.9, respectively.

a $t = 2.1(4)$ nm. The deviations of this model to the "as made" model may be due to magnetization of the Co, resulting in a higher Γ for the Co layers and roughness of the layers resulting in a (Gaussian) transition zone between two layers. Γ of the glass was also found to be higher, which can be due to uncertainties in glass composition.

3.2. *Without a priori knowledge*

A model was taken consisting of 10 layers of varying t and Γ. Four very different models were found all having a χ^2 less than or equal to 1.5. Two profiles are shown in Fig. 3 A ($\chi^2 = 1.2$) and B ($\chi^2 = 0.9$). Apparently with a fitting procedure based on genetic algorithms it is possible to find Γ's without any a priori knowledge fitting the data, stressing the nonuniqueness of the solutions. However, the models found in this way are hard to interpret and are likely to deviate largely from the model expected. By extending the q-range the measured reflectivity of the sample can deviate from the solutions found and the problem becomes less nonunique.

4. Conclusions

With genetic algorithms it is possible to find independent on experience of a neutron reflection expert an initial model for a least-squares fitting procedure. Without a priori knowledge about the sample it is possible to find scattering length density profiles that give good fits to the data, but are hard to interpret. Extending the measured q range will give extra information, excluding some profiles. With a priori knowledge about the structure of the sample, genetic algorithms can give different good fitting parameter sets of a model, where known information about the sample can give suggestions, which fit is "the" answer. Genetic algorithms in combination with a least-squares fitting procedure can be used as a tool to investigate the parameter dependence of the fit. It can find different sections of the parameter space where local minima are located. Because of the discreteness and mutation of the parameters it is not particularly suited to find local minima exactly, but in combination with a least-squares fitting procedure it is a powerful tool to fit neutron reflectivity data.

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