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Modelless approach in X-ray reflectivity of multilayer nanoheterostructure Fe / Cr

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Abstract

A new modelless method of determining the element concentration profile of metallic multilayer nanoheterostructures for low-contrast systems is applied to study periodical and aperiodical multilayer Fe/Cr system by X-ray reflectivity. As a special case, we discuss a cluster-layered Fe/Cr film with Kondo-like behavior of the resistance. The method does not require any a priori information on the structure of the multilayer nanostructures, such as position and width of interfaces as well as their shape. The method is based on solution of the Fredholm integral equation of the first kind, which relates the reflection coefficient and the concentration profile of the chemical elements of the sample. The ill-posed inverse problem of determination of the element concentration profile is solved by the regularization method. Efficiency of the method is confirmed by model calculations.

Keywords: X-ray reflectivity (XRR), multilayer structures, inverse ill-posed problem

1. Introduction

X-ray reflectivity (XRR) is now widely used to determine the structure and the composition of flat surfaces in the direction normal to a sample surface. The object of the reflectivity measuring is to determine the depth profile of electron density inside the material. Reflectivity data have been traditionally analyzed by trial-and-error and nonlinear least squares fitting methods using Parratt's recursive method of reflectivity calculation [1]. The main advantage of this method is that it involves relatively simple computation, but often, the result is rather subjective. It is known that in this case there is no stability and no uniqueness [2, 3]. The dependency of these fitting methods on an a priori postulated model finds its origin in the fact that normally only the amplitudes of the reflected waves are measured. Besides, these methods can not be applied to cluster-layered and aperiodic nanostructures because it is impossible to build a reasonable model in these cases.

Metallic multilayer nanoheterostructures are the films consisting of layers of various metals (often, 3d-neighboring elements like Fe, Cr), and each layer has a thickness from several angstroms to several nanometers. The particular interest to these materials has arisen after finding of their unique electric and magnetic properties, e.g., the effect of giant magnetoresistance (GMR) and Kondo-like behavior of the resistance for cluster-layered nanostructures [4].

Fe and Cr belong to a group of the 3d transition metals and their atoms have the similar electronic structure. It results in a small difference of the atomic scattering factors, and it is very difficult to distinguish these metals in the X-ray reflectivity experiment. This is the problem of low contrast.

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