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Mathematical model and computer simulation of three dimensional thin film elliptic interface problems

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ABSTRACT

Many engineering applications require information about temperature distribution in multilayer thin films. Steady state heat conduction in multilayer structures can be modelled by elliptic interface problems. In this paper, computer simulations of some thin film elliptic interface problems have been performed by applying decomposed immersed interface method on MATLAB.

1. Introduction

Thin films are thin material layers ranging from fractions of a nanometre to several micrometres in thickness. In past few years, thin films have become a major area of research because of its wide applications in engineering and technology. The calculation of temperature distribution in multilayer thin film structures is of interest in many fields e.g. X-ray lithography, magneto-optical (MO) recording, laser annealing, laser processing, electron beam lithography etc.

The phenomenon of steady state heat conduction in multilayer structures is governed by elliptic boundary value problems with interfaces, which are often called elliptic interface problems. The difficulty to solve such problems is caused due to the discontinuity across the interfaces. Discontinuity can be either in the solution or flux or the coefficient in the governing partial differential equations. Standard finite difference methods may not give accurate results for these problems especially near the interfaces because of the discontinuity.

The thin film elliptic interface problems arise in various industrial applications [1–10] e.g. X-ray lithography, used in the fabrication of micro-structures and devices with a high aspect ratio involves the irradiation of a photoresist on a substrate. An X-ray beam is transmitted through a multilayered structure containing a mask, a photoresist and a substrate having a gap between the mask and the resist. A mask, which is basically an X-ray absorber, creates a desired pattern on the photoresist by selectively allowing the transmission of irradiation from an X-ray beam. When the transmission is done, the photoresist, which is a light sensitive material, is developed to remove the irradiated area and an imprint of the pattern is left in form of exposed substrate and photoresist walls. This pattern is used as a micromold and it is filled with metal by electroplating. The remaining unexposed part of the photoresist is removed by an etchant and the desired microstructure is obtained on the substrate. Hence in the development of such microstructures, the knowledge of temperature distribution is required on the multilayered structure so that the effect of high flux X-ray exposure on distortions in the photoresist due to thermal expansion can be determined.

The solutions of such problems with usual methods are difficult to obtain because of three dimensional system and complex interface conditions between the different layers. Also, in the thin film system the width is much smaller than

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length and height; hence the resulting linear system becomes ill-conditioned. In many problems, we can have the elliptic equation with variable coefficient, which may lead to a non-symmetric linear system.

Previously some studies have been done regarding such type of problems by Dai and Nassar [1–7]. In [1] they have modelled an X-ray irradiated resist with three-dimensional heat equations and solved them by Douglas ADI method and the parallel "divide and conquer" scheme whereas in [2] the same model has been solved by applying a preconditioning technique and the Richardson method for the Poisson equation in the microscale and the tridiagonal linear system is solved by a domain decomposition algorithm based on the parallel "divide and conquer" scheme. Same type of problems with cylindrical geometry are modelled and solved in [3] using a hybrid finite element–finite difference method and a preconditioned Richardson method for solving the Poisson equation at the microscale. The resulting linear systems have been solved by a domain decomposing algorithm, obtained by applying a parallel Gaussian elimination technique. The same procedure is applied for solving a three dimensional heat transport equations in a double layered thin film with microscale thickness in [4] and for thermal analysis in X-ray Lithography in [5]. In [6,7], Dai and Nassar have solved different types of thin film problems by domain decomposition method.

In [8], temperature profiles produced in multilayered structure by laser or electron beam exposure are evaluated. The solution of coupled partial differential equations of thermal conduction has been calculated using Green's functions. The Green's function approach is also used to evaluate the analytical expression for temperature and probe beam deflection in multilayered structure in [9] and a local Green's function has been used to find out the solution of the heat conduction equation. The temperature and heat flux interfacial conditions have been used to link the local solution.

There are several methods in the literature [11–17] which can be applied to solve the thin film elliptic interface problem. In 1994, Li and LeVeque developed second order accurate immersed interface method [12] where they incorporated the jump conditions into the finite difference method. This method adds some additional nodes to the numerical stencil which may lead to a nonsymmetric matrix that is complex to be solved by standard numerical solvers. Hence the computational cost increases in solving such matrix.

In [11], a decomposed immersed interface method is presented where a correction term is introduced to standard difference stencil on the right hand side only so that the resulting linear system remains symmetric and diagonally dominant which can be solved by standard solvers. This correction term is decomposed in both cartesian directions. We have applied this method in multilayer thin film problems and computational results are discussed in graphical and tabular form in detail. Our motivation towards this work is the efficiency and robustness of this method for handling interfaces. We have also compared our approach with other existing techniques. The method is second order accurate, fast, efficient and easy to apply.

The remainder of the paper is constructed as follows: In Section 2 we have discussed mathematical model of a thin film elliptic interface problem arising in an X-ray irradiation process. In Section 3, we will discuss some other applications of thin film elliptic interface problems. In Section 4, we will explain the decomposed immersed interface method in detail. In Section 5, we have solved two thin film elliptic interface problems and performed their computer simulation and in the last section, we have summarized our work with some conclusions.

2. Mathematical model of a thin film elliptic interface problem arising in an X-ray irradiation process

In an X-ray irradiation process [1–5,7,8,10], the multilayered system contains a mask, a resist, a substrate and a gap between mask and resist which prevents overheating on the exposed area of the resist. The mask is generally made of gold or compounds of tantalum or tungsten, which absorbs X-ray. PMMA is generally used as the resist and it is placed on a substrate like silicon. All these layers including the gap are of microscale thickness. In an X-ray irradiation process this multilayered thin films structure works as a target of high flux X-ray beam as shown in Fig. 1. We need to study the effect of this X-ray exposure on resist.

First the heat is transferred through the mask by conduction. As the size of gap is very thin we can neglect the convection through the gap. Hence we assume that in every layer heat is transferred through conduction which can be modelled by the following elliptic equation:

$$-k_i\left(\frac{\partial^2 T_i}{\partial x^2}+\frac{\partial^2 T_i}{\partial y^2}+\frac{\partial^2 T_i}{\partial z^2}\right)=f(x,y,z), \quad i=1,2,3,4 \tag{1}$$

where k_i is the thermal conductivity and T_i is the temperature of ith layer. $f(x,y,z)$ is the source which can be determined by experiments. The boundary conditions are as follows:

On top surface. Heat convection occurs at top of the first layer i.e.

$$k_1\frac{\partial T_1}{\partial z}=h_c(T_1-T_\infty)$$

where T_∞ is the temperature of the surrounding and h_c is the convection coefficient.

At bottom surface of mask. The temperature and flux is continuous at the interface of mask and gap i.e.

$$T_1=T_2$$