The misfit stresses of dilatation line in semiconductor nanoheterostructures with angular boundaries

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Abstract. Misfit strains and stresses of a dilatation line in an elastic body with an angular free surface are studied with potential application to semiconductor nanoheterotechnology. The misfit stress fields in a wedge-shaped isotropic elastic space containing a dilatation line are calculated using the method of virtual surface dislocations and a Mellin transformation. Analysis of this solution is carried out numerically by using the misfit stress maps built in a cross section of the system.

1. Introduction

Studying the fields of misfit strains and stresses in semiconductor nanoheterostructures of complex architecture is an important problem for development of these nanoheterotechnologies. Differences in crystal lattices and thermal expansion coefficients of materials that compose nanostructure devices, significantly influence their work properties. Misfit stresses and residual thermoelastic stresses cause changes in the physical and service characteristics of the corresponding nanostructure devices. The relaxation of these stresses is accompanied by the formation of various defects, in particular, misfit dislocations, which also lead to degradation of device properties and shorten their service life. Therefore, the development of theoretical models of such defective structures is one of the key areas of fundamental research necessary for the development of modern semiconductor nanoheterotechnologies.

The solution of the boundary-value problems in the theory of elasticity allows us to study the features of the misfit stress fields at the stage preceding their relaxation, therefore, the formulation of such problems is an important initial stage in the development of theoretical models. In particular, one of such tasks is the search for elastic fields caused by dilatation inclusions with various shapes in an elastic body with an angular boundary. Such a boundary can be considered as a wedge-shaped protrusion or cut with an arbitrary opening angle. In this case, an infinitely thin dilatation line with its three-dimensional (3D) dilatational eigenstrain can serve as an elementary misfitting inclusion. Having a solution for such a line, it is possible to obtain by simple integration similar solutions for long inclusions with cross sections of arbitrary shape.

2. Methods and approaches

Consider an infinitely thin dilatation line embedded in an elastic body having the shape of a long straight wedge (figure 1). We assume that this line is subjected by a 3D dilatational eigenstrain, while its elastic moduli are the same as in the surrounding matrix. To solve this boundary-value problem, we use the method of virtual surface dislocations (VSDs).
Figure 1. Dilatation line in a wedge-shaped elastic body with free boundaries. The distribution functions $f_1$, $f_2$, $f_3$, and $f_4$ of virtual surface dislocations are sketched at the boundaries. $\alpha$ – wedge resolution angle, $\beta$ – angle by which the coordinate system rotates. $(x, y)$ – the coordinates of the dilatation line in the $xy$ coordinate system; $(x', y')$ – the coordinates of the dilatation line in the rotated coordinate system $x'y'$.

In the past, this method was successfully applied to various boundary-value problems of the theory of defects. In particular, similar problems were solved for edge dislocations in homogeneous [1] and composite [2] wedge-shaped bodies and screw dislocations placed near a triple junction of different wedge-shaped phases [3]. Within this method, the desired stress field is written as $\sigma = \sigma^\infty + \sigma^\nu$, where $\sigma^\infty$ is the well-known stress field of the dilatation line in an infinite elastic medium [4], and $\sigma^\nu$ is an extra stress field of the VSDs, continuously distributed over the free surfaces of the body in such a way that to ensure the fulfilment of traction boundary conditions on its angular boundary (figure 1).

In the present problem a dilatation line do is placed in a wedge with the angle $\pi/2 + \beta$ at its vertex and has coordinates $x = x_l$, $y = y_l$. To solve the boundary problem we introduce on each plane part of the boundary two distributions of virtual surface dislocations with Burgers vectors parallel and perpendicular to the surface, respectively, and use the well-known corresponding dislocation stress fields in an infinite medium [5]. Thus the resulting stress fields can be written in the form

$$\sigma_{ij}(x, y) = \sigma^\infty_{ij}(x, y) + \sum_{k=1}^{4} \int_{0}^{\infty} \sigma^k_{ij}(x, y, p)f_k(p)dp,$$

where $\sigma^\infty_{ij}(x, y)$ - are the stress fields caused by the dilatation line in an infinite medium and $\sigma^k_{ij}(x, y, p)$ ($k = 1$ to 4) are the stress fields of a probe surface dislocation located at a distance $p$ from the edge of the material and included in the $k$-th family. $f_k(p)$ denote the distribution functions of the surface dislocation densities. The boundary conditions $\sigma_{ij}n_i = 0$ can be written as $\sigma^\infty_{ij}n_i = -\sigma^\nu_{ij}n_i$, where $n_i$ is the $i$-th component of the normal vector on the surface.

In such a formulation, the problem is reduced to finding four unknown functions of distribution of the VSDs from the boundary conditions of the problem that gives a system of four integral equations.

$$\sum_{k=1}^{4} \int_{0}^{\infty} \sigma^k_{xy}(x - p, y = 0)f_k(p)dp = -\sigma^\infty_{xy}(x, y = 0)$$

(2a)
The results is a system of four algebraic equation for the transformed distribution functions obtained using the Mellin integral transform

\[ \tilde{f}_k(s) = \int_0^\infty f_k(p) p^{s-1} dp, \]  

where \( s \) is a complex variable. The some integrals from equation (2) with the substitution of equation (3) are given in [6].

Further the problem is to calculate the distribution functions using the back transformation

\[ f_k(p) = \frac{1}{2\pi i} \int_{\varepsilon-i\infty}^{\varepsilon+i\infty} \tilde{f}_k(s) p^{-s} ds, \]  

where \( \varepsilon \) is a real part \( s \). The resulting stress fields \( \sigma_{ij} \) can be written as

\[ \sigma_{ij} = \sigma_{ij}^{\infty} + \sum_{k=1}^{4} \frac{1}{2\pi i} \int_{\varepsilon-i\infty}^{\varepsilon+i\infty} \tilde{f}_k(s) \lambda_{ij}^k(x, y, s) ds, \]  

where

\[ \lambda_{ij}^k(x, y, s) = \int_0^\infty \sigma_{ij}^k(x, y, p) p^{-s} dp \]

The analysis of the obtained solution was carried out numerically using the stress maps built in the cross section of the system.

3. Results
An investigation of the symmetry properties of the integrands in equations (2) leads to a simplification: since the imaginary part of \( f_k \lambda_{ij}^k \) in equation (5) is antisymmetrically with respect to \( \text{Im}(s) \) it vanishes after integration. The real part is symmetrically, and therefore the integration can be simplified. The integrals were calculated using a generalized Simpson rule in an \( \text{Im}(s) \)-range from 0 to 50 with about 1000 intervals and \( \text{Re}(s) = \varepsilon = 0.7 \). The convergence of the integrals, the fulfilment of the boundary conditions, and the independence of the integrals of \( \text{Re}(s) \) in the range \( 0.5 < \text{Re}(s) < 1 \) were controlled numerically.
Figure 2. Stress maps of a dilatation line in a wedge-shaped elastic body in units of $Gb/(2\pi L(1-\nu))$. $L$ is the unit of length on the coordinate ($G = 40$ GPa, $\nu = 0.35$). $\sigma_{xy}, x_l = 3L, y_l = L, \beta = 45^\circ$.

An example of the dilatation line stress fields near a wedge-shaped surface is represented in figure 2, where the equistress curves are plotted for the component $\sigma_{xy}$. This map (figure 2) showed, in particular, that the boundary conditions of the problem are satisfied with good accuracy. Positive stresses decrease with distance from the dilatation line, and negative stresses increase.

4. Summary and Conclusion
In the present work, the method of virtual surface dislocations (VSDs) is used to find a solution of the boundary-value problem in the theory of elasticity for a dilatation line embedded in an elastic body with an angular boundary. The solution is found as a superposition of the well-known stress field of the dilatation line in an infinite elastic medium [4] and an extra stress field of the VSDs (equation (1)). The latter is given by the inverse Laplace-Mellin transform of the products of the Mellin images of the stresses of individual VSDs and their distribution functions (equation (4)). With this solution on hand, one can obtain by simple integration similar solutions for long inclusions of arbitrary-shape cross sections in various semiconductor nanoheterostructures.

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