Boundary-value problems for defects in nanoscale and nanocomposite solids

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Abstract A brief review of solutions of boundary-value problems in the theory of elasticity for defects in nanoscale and nanocomposite solids, which were found during the last three decades in the Laboratory of Mechanics of Nanomaterials and Theory of Defects at the Institute for Problems in Mechanical Engineering of Russian Academy of Sciences, is presented. It covers the elastic behavior of dislocations, disclinations and inclusions near free surfaces and interfaces in such inhomogeneous nanostructures as composite nanolayers, core-shell nanowires and nanoparticles, quantum dots and wires in subsurface layers, etc. Some relevant works dealing with application of the solutions found to the theoretical models describing the nucleation and development of different defect structures in the process of crystal growth and misfit stress relaxation in advanced composite nanostructures which are highly promising for use in modern electronics, optoelectronics and photonics, are also briefly reviewed.

1 Introduction

In the present paper, we give a brief review of solutions of boundary-value problems in the theory of elasticity for defects in nanoscale and nanocomposite solids, which were found and used during the last three decades in the Laboratory of Mechanics of Nanomaterials and Theory of Defects at the Institute for Problems in Mechanical Engineering of Russian Academy of Sciences (IPME RAS). These solutions were given within isotropic elasticity for straight dislocations and disclinations, circular

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and rectangular dislocation loops, circular disclination loops, inclusions of different shapes, sharp and diffuse interfaces in elastic solids bounded by planar, cylindrical and spherical free surfaces, and in inhomogeneous elastic solids with planar, cylindrical and ellipsoidal interfaces. The results normally included the displacement and stress fields of the defects, their strain energies and sometimes the interaction energies of the defects, and elastic image forces acting on the defects from the free surfaces and/or interfaces. These results were extensively applied to theoretical models describing misfit strain/stress relaxation and defect generation in various solid-state micro- and nanoheterostructures which are the basis of advanced structural and functional materials. Some of these solutions and results were reviewed in more detail in monographs [1, 2] and reviews [3–10]. In most cases, our results were obtained within the classical theory of elasticity and this will not be specially noted anymore, although sometimes the gradient elasticity and the surface/interface elasticity were used as well. In both the latter cases, we will specially announce about. We devote this brief review to the 30 anniversary of IPME RAS.

2 The method of virtual surface defects in the solution of boundary-value problems of the theory of defects

Elasticity boundary-value problems for defects of different dimensionality, i.e. for point, line, surface, and volume defects, with prescribed geometrical characteristics, e.g. configuration of dislocation line, or inclusion shape, located in the bodies with various geometries, were solved analytically both by standard methods of mathematical physics and theory of elasticity (see, e.g. [11, 12]) and by a new method of virtual surface defects (MVSD) that was advanced for the solution of such problems.

In the framework of the MVSD, which is further development of surface straight-linear dislocation-disclination technique [13–17], virtual defect types are chosen according to the symmetry of the boundary-value problem for real defect under consideration. Virtual defects are then continuously distributed on free surfaces or/and interfaces in such a way that their elastic field together with the field of the real defect satisfy the imposed boundary conditions. In works [18–20], defect loops (including Volterra and Somigliana ring dislocations) were proposed as virtual defects for solving elasticity boundary-value problems with axial symmetry. Defect ring loops were defined as planar defects with the *eigenstrain* prescribed in the part of the plane bounded by a circle [21,22].[1] A characteristic feature of the elastic fields of the circular (ring) loops is a possibility to express their fields though Lipschitz-Hankel integrals [23] that is extremely convenient because of separation of axial and radial variables.

Boundary conditions accounting for the distributed virtual loops acquire the form of integral equations for unknown distribution functions which are solved by

[1] Note that only Volterra dislocations, i.e. translation (ordinary) dislocations and disclinations, can be considered as linear (1D) defects as a degenerate case of more general class of surface (2D) defects – Somigliana dislocations [22].

the integral transformations. For the case of the planar boundaries, Hankel-Bessel transform is used, see, e.g. [24, 25]; for the case of cylindrical boundaries – Fourier transform [25,26]; and for the case of spherical surfaces, the expansion of the elastic field components of virtual defect loops in the series with Legendre polynomials is used [27]. When discussing below the results of our studies, MVSD is presented in necessary details and variety.

3 Dislocations

General reviews on the boundary-value problems for dislocations in the classical theory of elasticity were given by Dundurs [28], Eshelby [29], Lothe [30] and Belov [31]. A great number of more recent solutions are spread over original papers, from which we will consider the works of our lab only.

3.1 Straight dislocations

3.1.1 Edge dislocations

Gutkin and Romanov [32, 33] considered an edge dislocation parallel to the surfaces in a thin two-layer film with different elastic moduli. The solution was obtained in the integral form using a modernized MVSD, i.e. using the fields of both the considered dislocation and virtual surface dislocations, which satisfy the boundary conditions on the interface [32]. It was shown [33] that the dislocation may have from one to five equilibrium (stable and unstable) positions in the film interior, depending on the Burgers vector orientation and the ratio between elastic moduli of the layers. These results were later applied to some related problems, the first of which were the models of misfit dislocations (MDs) in similar systems with lattice mismatch of the layers [34,35]. The strain energy of the dislocation found in [33] allowed to define the critical conditions for nucleation of MDs and their stable positions near the interface. It was shown that, depending on the parameters of the two-layer film, a MD may occupy the stable equilibrium position in the softer layer (the so-called 'stand-off position') or directly in the interface. More recently, the stress fields and strain energy found in [33, 34] have been used in the models describing the critical conditions for the formation of MDs in core-shell nanoparticles (NPs) [36]; the glide of circular prismatic [37, 38] and mixed [39, 40] dislocation loops along the interface between straight [37, 38] or Y-shaped [39, 40] nanotubes (NTs) and ceramic matrix at the bridging [37, 38] or pull-out [39, 40] stages of fracture in ceramic nanocomposites; and the emission of dislocation dipoles from an edge of a long prismatic nanowire (NW) of rectangular cross-section embedded in a free-standing nanolayer [41].

Using Romanov's [42] solution for the Airy stress function of an edge dislocation (as a limiting case of a biaxial dipole of wedge disclinations) in an elastic cylinder, Gutkin et al. [43] for the first time considered the generation of a straight edge MD in a core-shell NW. The formation of the MD in such a NW was assumed to be driven by the misfit stresses associated with the mismatch of the lattice parameters of the core and the shell. It was shown that the generation of the MD decreases the strain energy of the system and can be realized at some ranges of parameters (misfit, core radius and shell thickness). To calculate the conditions for the formation of a straight MD parallel to the NW axis, Gutkin et al. [43] first calculated the misfit stresses and then cast the conditions at which the MD generation is energetically beneficial. It appeared that the MD generation is favored if the thicknesses of both NW phases (the core and the shell) are not too small. Also, according to [43], the generation of an MD requires that the misfit should be large enough and the core radius and shell thickness should be not too different. The calculations [43] also predict that a decrease in the core radius makes the generation of a straight MD more difficult. This situation is similar to the case of MDs in films on planar substrates, where a decrease in the substrate thickness also hinders the formation of MDs at or near the film/substrate interface [44, 45].

The theoretical analysis of MD formation in NWs was complemented by the analysis of their generation in uncapped islands and NWs on the surface of a thick substrate or on the surface of a thin film layer located on a substrate. For example, theoretical models describing the formation of partial, split and delocalized dislocations in NWs on the substrate surface were suggested in Refs. [46–48]. The first of these models [46] considers a composite solid consisting of a semi-infinite crystalline substrate and a pyramidal crystalline island modeled as a triangular NW. In this case, the author approximated the self-strain energies and the interaction energies of MDs by the solutions found for edge dislocations parallel to the flat free surface of a half-space [28, 29]. In contrast, in Refs. [47, 48], the substrate and the island were modelled as cylindrical segments that together composed a cylinder, in which case the authors used the Airy stress function [42] as the departure point. As with model [46], 2D models [47, 48] describe dislocations in a 2D NW. However, their results can be extended to the case of 3D islands.

The calculations performed in Ref. [47] demonstrated that near an island edge the most energetically favorable dislocation structure is a single partial MD. During the motion of this MD inside the island, the nucleation of a second partial MD at the island edge and its motion along the substrate-island interface become favorable. The motion of partial MDs may happen until they have reached their equilibrium positions located symmetrically at opposite sides from the island base centre. In parallel with localized dislocations, the formation of dislocations delocalized over a strip of a certain width can occur in islands [48]. The calculations [48] showed that the energy of a delocalized dislocation in an island is always smaller than the energy of a localized one. As a result, the nucleation of a delocalized dislocation in an island may occur even in small islands, where the formation of conventional localized dislocations is energetically unfavorable.

Recently, Smirnov et al. [49] have used the solution [42] for an edge dislocation in a cylinder for analyzing the mechanisms of misfit stress relaxation in core-shell NWs, in which the cores had the shape of long prisms of square cross sections.

In particular, they have shown that the emission of dipoles of partial and perfect dislocations by edges of the cores are the most energetically favorable relaxation mechanisms in relatively thin and thick NWs, respectively.

Besides the solutions obtained within the classical theory of elasticity, some boundary-value problems were also solved for edge dislocations within the gradient elasticity [50] and the surface/interface elasticity [52–56]. Mikaelyan et al. [50] used one of the early versions of the stress/strain-gradient elasticity, first suggested by Ru and Aifantis [51], to obtain a solution of the boundary-value problem for a straight edge dislocation parallel to the planar interface between two elastic isotropic media with different elastic constants and different gradient coefficients. The main difference of this gradient solution from the classical one [11] is that the dislocation stress field has no singularities on the dislocation line and remains continuous at the interface, while the classical solution is singular at the dislocation line and allows a discontinuity of two stress components at the interface. The gradient solution also removes the classical singularity of the image force for the dislocation on the interface. Moreover, an additional elastic image force associated with the difference in the gradient coefficients of contacting phases was determined. It was shown that this force, which has a short range and a maximum at the interface, expels the edge dislocation into the material with a smaller gradient coefficient.

The surface/interface elasticity was used to reveal new nanoscopic peculiarities in elastic behavior of edge dislocations inside the wall of a nanotube [52], near an elliptical nano-inhomogeneity [53], in a core-shell NW embedded to an infinite matrix [54] as well as in the shell of a free-standing core-shell NW [55]. Based on the results of these work, one can conclude that there is no special need to use the more complicated surface elasticity theory for describing the dislocation fields and behavior in the bulk of a nanoscale solid at distances larger than about 1 nm from the free surface or the interface. When studying the situation near the free surface or the interface, the choice between the classical and surface theories of elasticity depends on the values of surface elastic moduli. On the other hand, the non-classical effects in nanoscale solids can be very impressive. For example, in the case of an edge dislocation placed in the shell of a core-shell NW, these effects are [55]: (i) the stress oscillations along the shell surface and core-shell interface for negative values of the surface/interface elastic moduli; (ii) a strong dependence of image forces on the core size; (iii) extra repelling (attraction) of the dislocation from (to) the shell surface and core-shell interface characterized by positive (negative) interface modulus; and (iv) a decrease of the dislocation strain energy in the central region of the shell and its local increase with an extra maximum in the vicinity of the shell surface for negative values of the surface/interface elastic moduli. Moreover, the study of the surface/interface effects on the formation of MDs in a core-shell NW showed [39] that these effects are significant for fine cores of radius smaller than roughly 20 interatomic distances. The positive and negative surface/interface Lamé constants mostly make the generation of the MD easier and harder, respectively. The positive (negative) residual surface/interface tensions mostly make the generation of the MD harder (easier).

3.1.2 Screw dislocations

For screw dislocations, a number of boundary-value problems have been solved in our lab within the classical, gradient and surface/interface theories of elasticity. Some of these problems concern 'normal' screw dislocations with full cores, while the others deal with 'abnormal' hollow-core screw dislocations which are commonly referred to as 'micropipes' (MPs). First, we will consider the solutions done for normal screw dislocations, and then turn to MPs.

Gutkin et al. [57] solved the problem of a screw dislocation placed near a triple junction of flat interfaces separating phases with different elastic moduli. In doing so, they used the modernized MVSD method similar to that suggested by Gutkin and Romanov [32]. The exact analytical expressions for the dislocation stress fields were found in the Mellin space in the general integral form. For the limiting case, when the interphase boundaries contacted under right angles, the Mellin transforms for the functions of distribution of virtual surface dislocations were represented in the closed explicit form.

Gutkin and Sheinerman [58] analyzed the elastic behavior of a screw dislocation in the wall of a hollow NT. They used the method of infinite image-dislocation rows [59] and represented their solutions for the stress fields, strain energy and image force by infinite series convenient for numerical analysis. The internal space of the NT was shown to cause (i) a change in the sign of stress-tensor components near the inner NT surface, (ii) a high stress concentration and (iii) a strong stress gradient at this surface. It was also shown that the dislocation has one position of unstable equilibrium in the NT wall, which is always shifted toward the inner NT surface. As the internal-space radius increases, the dislocation energy decreases and the position of its equilibrium shifts toward the outer NT surface; in the limiting case of a flat layer, it reaches the center of the layer.

The technique of infinite arrays of image dislocations was also used [60] to calculate the stress field and strain energy of a screw dislocation in an elastically isotropic solid containing two cylindrical voids. Based on the solution derived, the image force exerted by the two voids on a screw dislocation was also calculated and studied. As a limiting case of the solution obtained, the authors derived the stress field of a screw dislocation in a half-space containing a cylindrical void. It was shown, in particular, that, if the void radii are smaller than their spacing from the dislocation, the voids significantly influence the dislocation stress fields at the distances of several void radii from the void surfaces.

Kolesnikova et al. [61] solved the boundary value problems for screw dislocations normally piercing two-layer flat film and two-layer hollow sphere. The analytical solutions were found by the MVSD. Elastic fields of the dislocation in the film were presented in the form of integrals with Bessel functions, while those of the dislocation in the hollow sphere in the form of series with Legendre polynomials. The stress fields were analyzed by stress maps which allowed to reveal some peculiarities in stress distribution in dependence of the geometric and elastic parameters of the systems. It was demonstrated that in the limiting cases of a homogeneous plate and a half-space, the solutions for a screw dislocation coincide with the solutions found by the authors earlier [18, 19], as well as with the solutions the first given by Eshelby and Strogh (plate) [62] and Yoffe (half-space) [63] and found with other techniques. When passing from a two-phase spherical layer to a solid sphere, the fields of a screw dislocation become fields first derived by Polonsky et al. [64], and after that recalculated with the MVSD [27].

Gutkin et al. [65, 66] found the solution for a screw dislocation parallel to the planar interface between two elastic isotropic media with different elastic constants and different gradient coefficients within the stress/strain-gradient elasticity [51]. The principal differences from the well-known classical solution [28] are practically the same as in the case of an edge dislocation (see above Subsection 3.1.1).

Shodja et al. [67] used the simplest strain-gradient elasticity theory [68] to analyze the displacement and strain fields of a screw dislocation in a free-standing NW. They showed that these fields do not contain classical jumps and singularities at the dislocation line. Moreover, the maximum values of the displacement and elastic strain strongly depend on both the dislocation position and NW radius, thus demonstrating a nonclassical size effect.

Davoudi et al. [69, 70] considered the cases of a screw dislocation inside [69] and near [70] an embedded NW within the gradient elasticity theory suggested in [51]. In both the cases, the classical stress singularity was removed from the solutions and all stress components were continuous and smooth across the interface, in contrast with the results obtained within the classical theory of elasticity [28]. As a result, the image force exerted on the dislocation due to the differences in elastic and gradient constants of the matrix and NW, remained finite when the dislocation approaches the interface. The maximum magnitude of dislocation stress greatly depended on the dislocation position, the NW size, and the ratios of shear moduli and gradient coefficients of the matrix and NW materials.

The surface/interface effects on elastic behavior of a screw dislocation in finite-size and inhomogeneous nanostructures were studied in Refs. [71–73]. Shodja et al. [71] studied the same case of a screw dislocation inside the wall of a NT as Gutkin and Sheinerman [58] within the classical elasticity. The non-classical results demonstrated [71] that in tiny NTs with wall thickness in the order of a few nanometers, the surface stresses noticeably affect the bulk stress fields over the NT's cross section, while in coarser NTs, the surface stress effect is negligibly small. Further, a screw dislocation was repelled by the inner and outer free surfaces, which is an atypical behavior in the context of classical elasticity. Thus, a screw dislocation had one unstable equilibrium position in the bulk of the NT wall, as is also the case with the classical elasticity [58], and additionally two stable equilibrium positions in close vicinity of the free surfaces. However, this non-classical effect was strictly localized in atomically thin subsurface layers. It was also shown that the image force strongly depends on the NT radii and elastic characteristics of the surfaces.

Ahmadzadeh-Bakhshayesh [72] analyzed the surface/interface effects for a screw dislocation in an eccentric core-shell NW. They showed that (i) near the free surface and the interface, the stress fields considerably differ from the classical ones, while this difference practically vanishes in the bulk of the NW; (ii) the surface with positive (negative) shear modulus applies an extra non-classical repelling (attracting) image force to the dislocation, which can change the nature of the equilibrium positions depending on the system parameters; (iii) the non-classical surface/interface effect has a short-range character and becomes more pronounced when the nanowire diameter is smaller than 20 nm.

Shodja et al. [73] considered the interface effect on the critical condition for the formation of a screw misfit dislocation dipole (MDD) at the interface between an embedded NW with uniform shear eigenstrain field and surrounding matrix. The critical radius of the NW corresponding to the MDD generation was shown to decrease with the increase in the uniform shear eigenstrain inside the NW as well as when the stiffness of the NW increases with respect to the matrix, and to strongly depend on the non-classical interface parameter.

In addition to boundary-value problems for full-core screw dislocations, the studies of our lab included the investigations of the elastic behavior of MPs which are in fact hollow-core superscrew dislocations with giant Burgers vectors often observed in some crystals with hexagonal crystalline lattice, for example, in silicon carbide [74]. The first of these works [75] considered the elastic interaction of a dislocated MP with a screw dislocation or another dislocated MP. For the analysis of the elastic interaction between MPs, the stress field of a dislocated MP in the solid containing another MP was derived using the technique of infinite arrays of image dislocations [59]. The stress field, strain energy and the force of interaction of two MPs, the parameter regions where they are attracted or repelled were determined. It was demonstrated that at distances large as compared to the radii of the MPs, the presence of MP free surfaces can be neglected, and the interaction force between MPs approaches that of two dislocations in an infinite medium. That is, in this case, the MPs with opposite-sign Burgers vectors attract each other, while those with same-sign Burgers vectors repel each other. At the same time, when the distances between the MPs are short enough, the contribution of the MP free surfaces to the interaction force may dominate. As a consequence, for same-sign MPs, there exists a parameter region where they attract each other. The attraction area for such MPs exists if the ratios of their radii and Burgers vectors magnitudes are sufficiently different.

Using the expression for the energy of a pair of MPs, the criterion for MP split into two smaller MPs has been derived [76]. With the assumption that the split is possible if the energy of MPs after the split is smaller than the energy of the initial MP, it was shown that the MP split is energetically favorable in a certain parameter region if the MPs are of the same sign. The parameter region comprises the normalized magnitudes of the Burgers vectors as well as the radii of the initial and split MPs. This region expands if the radius of the initial MP rises. The split of an MP into two smaller ones is possible if the radius of the initial MP exceeds the equilibrium radius and the total MP surface energy decreases due to the split. The MP split also requires that the ratio of the split MP radii should be close to that of the magnitudes of the MP Burgers vectors.

In works [75,76], it was supposed that the MPs are situated in an infinite medium. However, the split of an MP is also likely to happen at the crystal growth front. For example, in work [77] the split of a MP into another MP and a full-core screw dislocation has been proposed to occur through the lateral motion of the surface step produced by the MP. In terms of the dislocation theory, the split of an MP at or near the crystal growth front may be considered as the formation of a glide dislocation semi-loop. Since such a split occurs near the crystal free surface, its theoretical analysis required preliminary solving a number of boundary-value problems for the MPs terminated at the free crystal surface.

The first of these problems was the problem about an MP perpendicular to a free crystal surface [78]. The exact analytic solution of this problem was obtained with an account for both the cylindrical surface of the MP and its perpendicular flat crystal surface. The displacement, strain and stress fields of the MP in a half-space were calculated in [78] through distributing virtual twist disclination loops over the MP surface. As a result, it was demonstrated, in particular, that the rigorous account for the boundary conditions at the cylindrical MP surface considerably influences the stress field of the MP. The region of strong influence is situated around the MP at the distance of the order of the MP radius. In this region, the elastic strains may reach high enough values of several tenths of a percent.

Another boundary-value problem whose solution is necessary for the analysis of the MP split near the crystal free surface is the problem on glide rectangular dislocation loops that are perpendicular to a free surface. The energy of such dislocation loops was calculated in [79] using the Green function method.

Using the obtained solutions of the boundary-value problems for the MP and dislocation loops perpendicular to a free surface, Gutkin and Sheinerman [79] carried out a theoretical analysis of the MP split into a smaller MP and a dislocation semi-loop. The calculations demonstrated the existence of the MP attraction zone (with the width of several hundredths to tenths of MP radius) and the flat crystal surface attraction zone (with the width of several MP radii), which the semi-loop has to overcome before its expansion becomes energetically favorable. The semi-loop can pass over the flat crystal surface attraction zone owing to the crystal growth, while going through the MP attraction zone requires the presence of an external perturbation or a stress source. After the semi-loop has left the attraction zones, it becomes stable, and the MP split becomes irreversible. Thus, a fast crystal growth may get it easier for the semi-loop to pass over the attraction zone and thereby promote the split of an MP (provided that the split has already been initiated due to an external perturbation or a stress source). Therefore, one may suppose that MPs are most likely to split and be overgrown if the crystal growth rate is sufficiently high.

Gutkin and Sheinerman [79] also theoretically showed that the most expectable trajectory of the semi-loop central point goes rather closely to the MP in such a manner that the shape of the semi-loop becomes strongly elongated along the MP. Therefore, the new MP, which may be formed around the semi-loop line, has to lie just near the initial MP. This conclusion is in good agreement with the experimental observations of ramifying MPs in silicon carbide [76].

Another boundary-value problem solved for the MPs concerns the calculation of the elastic fields of MPs with axially symmetric steps [80]. The evidence of such steps is clearly demonstrated by scanning electron microscopy observations of MPs appearing at the free surface of a crystal (see, for example, [76]). In view of the presence of the sharp step edge, such a problem cannot be solved using traditional methods of dislocation theory. However, its approximate but fully analytical solution was obtained [80] using the method [81] for studying the effect of stress concentration near rough surfaces. Gutkin and Sheinerman [80] considered separately MPs that lie in an infinite medium and MPs perpendicular to a planar free surface. For both the cases, they calculated the thermodynamic forces acting on the steps. For MPs in an infinite medium, the force of interaction between their steps was also found. For an MP with a step, perpendicular to a free surface, the equilibrium position of the step was estimated. It was shown that subsurface MP steps repulse from the free surface if they result in decreasing the MP radius. This means that, in vicinity of the free surface, the MP radius may reduce compared to its radius far from the free surface if the energetic barrier for the generation of subsurface steps is overcome. It was also shown that same-sign steps attract each other (at least, as long as they are small), and so the formation of large enough steps at the MP surface is possible.

It is worth noting in conclusion that the solution for a screw dislocation interacting with two cylindrical voids [60] was used to describe the effect of contact-less reaction of two MPs by exchange of full-core screw dislocations that should lead to diminishing the radii of reacting MPs and potentially to their healing in the growing crystal [82, 83]. This theoretical model was supported by experimental observations combined with computer simulation of the phase contrast images of MPs obtained in X-ray synchrotron radiation [82, 83].

3.2 Dislocation loops

In real materials and solid-state structures, dislocations often form closed loops of various shapes [59]. Dislocation loops are of special interest for theoretical models dealing with nucleation and multiplication of dislocations. In our lab, a number of boundary-value problems have been solved for circular and rectangular dislocation loops with some application to the models of MD generation in core-shell NPs and NWs, quantum dots (QDs), and stress relaxation in pentagonal NPs and whiskers.

For example, the problem of a circular prismatic dislocation loop (CPDL; ‘prismatic’ means that the Burgers vector of the loop is normal to its plane, in contrast to ‘glide’ dislocation loop with its Burgers vector parallel to the loop plane [59]) placed in the axisymmetric position in the cross section of a long elastic circular cylinder, was solved independently by Ovid’ko and Sheinerman [84], Aifantis et al. [85], and Chernakov et al. [86]. The authors used different techniques and found different mathematical forms for their solution, however the aim was in general the same: to analyze the critical conditions for the generation of MDs in core-shell NWs. Indeed, besides the formation of straight MDs, the relaxation of misfit stresses in core-shell NWs is possible via the formation of MD loops at the NW cross sections. It was found that the formation of a CPDL is energetically favored if the misfit exceeds a critical value. This critical misfit decreases with an increase in the core radius or shell thickness, similar to the case of the nucleation of a straight MD. For a specified misfit, the formation of a CPDL in a core-shell NW is beneficial if the core radius and the shell thickness are not too small. Chernakov et al. [86] also calculated the energy of elastic interaction between two similar CPDLs and used this result to determine the equilibrium density of such CPDLs in a core-shell NW. In the special case of the InAs-GaAs core-shell NW of diameter 100 nm and core-shell radii ratio ~0.7, experimentally grown and studied by Popovitz-Biro et al. [87], the authors [86] showed that the calculated equilibrium spacing of misfit CPDLs 8.35–9.05 nm was in good agreement with their experimentally observed spacing 7.0–8.5 nm. The relative energy gain caused by such partial misfit stress relaxation was estimated as roughly 31%.

Another research topic of the lab comprised the analysis of dislocation behavior in nanocomposites containing capped or uncapped islands (QDs) or NWs. One such a model considered a misfit CPDL around a subsurface cylindrical QD [88]. Such a QD represented an inclusion in the form of a finite-height cylinder situated in a film on a semi-infinite substrate. The flat facet of the QD was supposed to enter a surface of a semi-infinite matrix. To calculate the conditions for the CPDL formation, the authors used the well-known strain energy of the CPDL near a flat free surface and its stress fields [89] for finding the energy of elastic interaction of the CPDL and the QD. Their theoretical analysis [88] demonstrated that the formation of a CPDL around a subsurface cylindrical QD of a specified height is easiest if the diameter of this QD is approximately equal to its height and becomes more difficult with an increase of the absolute difference between the QD diameter and its height.

In the work [20], Kolesnikova and Romanov presented elastic fields of CPDL located parallel to the free surfaces of a flat plate. This solution was found using MVSD, in which two types of circular loops were chosen as virtual defects: CPDLs and the radial Somigliana dislocation ring loops [18–20].

Kolesnikova et al. [90] solved the boundary-value problem for an axially symmetric CPDL in an elastic hollow sphere. They calculated the stress fields and the strain energy of the CPDL and showed that the CPDL stress and dilatation fields are strongly screened and distorted by the free surfaces of the sphere as compared with the case of a CPDL in an infinite medium. Moreover, they revealed some interesting qualitative peculiarities in the distribution of the elastic fields, which would be impossible to predict based on the infinite-medium solution. This mainly concerns the CPDL dilatation which can change its sign in the subsurface layers of the particle, near the cavity and in the shell. In the case of an interstitial CPDL, some regions of 3D stretching appear near the free surfaces where the conditions favorable for surface nucleation of vacancies are formed. These vacancies are stimulated to migrate to the interstitial CPDL, accommodate the compression near it and annihilate with the interstitials forming the CPDL. As a result, the CPDL can be kinetically unstable in the systems under discussion. On the other hand, the interstitials and impurities having the atomic size larger than that of the parent atoms, are stimulated to migrate to the stretched regions and form their surface segregations or even second phases. The strain energies of CPDLs were shown to strongly depend on their radii and positions in particles and shells, or near cavities. In particles and shells, the strain energy reaches its maximum when a CPDL lies in the equatorial planes and has the radius of roughly 0.8 of the particle radius or outer radius of the shell, if the latter is several times larger than the inner radius of the shell. For a cavity, the strain energy of a CPDL increases with its radius and its shift from the equatorial plane.

The solution [90] was extensively used in recent years for theoretical modeling of stress relaxation in bulk [91, 92] and hollow [92, 93] core-shell NPs, icosahedral [94] and decahedral [95] small particles, decahedral core-shell NPs [96] and core-shell nanoparticles with truncated spherical cores [97]. Moreover, Krasnitckii et al. [98] utilized this solution to calculate the energy of elastic interaction of two coaxial CPDLs in an elastic hollow sphere. They showed that the interaction energy of CPDLs is strongly screened by free spherical surfaces when at least one of the CPDLs is localized near the surface. The outer free surface makes a greater effect on the interaction energy than the inner free surface. In particular, there is a region near the equator and the outer free surface, where the interaction energy changes its sign. The inner free surface does not give such effect.

Besides the CPDLs, the rectangular prismatic dislocation loops (RPDLs) have also been in the focus of research in our lab. For example, Gutkin et al. [99] analyzed the critical conditions for the formation of various misfit defects at the interface between subsurface NWs of rectangular cross section, which were parallel to a free surface, and surrounding semi-infinite matrix. It was supposed that the accommodation of the misfit stresses in such a system might occur through the generation of either RPDLs, or dislocation semi-loops, or dipoles of straight MDs. The defects were supposed to form if their generation was energetically favorable. For the calculation of the strain energy of the RPDL, the authors applied the Green function method. The calculations [99] demonstrated that taking into account of the NW shape anisotropy and the presence of a free surface nearby significantly alters the critical conditions for defect formation in a NW. In contrast to cylindrical NWs and spherical QDs in an infinite medium, an increase of one of the sizes of a subsurface rectangular NW does not always reduce the critical misfit for the formation of RPDLs, although it decreases the critical misfit for the formation of MD dipoles at the NW-matrix interface. The presence of a matrix free surface may either increase or decrease the critical misfits for the nucleation of RPDLs and MD dipoles.

The strain energy of a RPDL placed normally to a close flat free surface, found in [99], were recently used in theoretical models of initial stages of misfit stress relaxation in various composite nanostructures of spherical (bulk [92, 100, 102] and hollow [92, 101, 102] core-shell NPs), cylindrical (bulk [101–105] and hollow [101, 102] core-shell NWs) and flat (bi- and tri-nanolayers [101, 102]) geometry. Based on the strained states in the misfitting nanostructures, the authors quantitatively estimated changes in their energies, which accompany the generation of RPDLs in them, revealed places of the energetically more favorable generation of the RPDLs in these nanostructures and determined optimum shape of the RPDLs. By comparing the critical conditions for appearance of the most energetically favorable RPDLs in the different composite nanostructures, Gutkin and Smirnov [101, 102] ranged the relative stabilities of these nanostructures against generation of RPDLs. In particular, they showed that the hollow nanostructures are always more stable than their bulk counterparts, the cylindrical nanostructures are more stable than the symmetric flat tri-nanolayers, the spherical nanostructures are more stable than the cylindrical ones, and the flat bi-nanolayers are the most stable composites among those under investigation.

4 Disclinations

For disclinations, quite a limited number of boundary-value solutions have been found in our lab, although some earlier solutions were used in theoretical modeling. In particular, in parallel with MDs, other misfit defects can nucleate in core-shell NWs. An example is wedge disclinations (WDs) that can form at the junctions of twin or grain boundaries in poly- and nanocrystalline solids [9, 28, 106]. The elastic solutions, found by Romanov [42] for WDs in elastic cylinder, were applied by Sheinerman and Gutkin [107] to examine the critical conditions of the formation of individual misfit WDs, their dipoles and arrays in core-shell NWs. In considering individual misfit WDs, the authors showed that their appearance at the core-shell interface is energetically favored if their strength is smaller than a critical strength. In contrast, the formation of a WD dipole, with one WD at the core-shell interface and another inside the shell, is beneficial if the disclination strength exceeds another critical strength. Similar to individual misfit WDs, the formation of a periodic array of misfit WDs at the core-shell interface is favorable if the disclination strength is below some critical strength that depends on the core to NW radii ratio, misfit and the number of misfit WDs in the array.

Another example is the solution for a bi-axial dipole of WDs in a thin elastic layer [16], which was used by Dynkin and Gutkin in their models of stress-coupled migration of grain boundaries in ultra-thin nanocrystalline films under tension [108, 109].

New solutions were found by Shodja et al. [110] for a bi-axial dipole of WDs in an embedded NW and by Rezazadeh-Kalehbasti et al. [111] for a bi-axial dipole of WDs and an individual WD in the shell of a free-standing core-shell NW. In both the cases, the surface/interface elasticity was used. Shodja et al. [110] showed that the positive interface modulus leads to increased strain energy and extra repulsive forces on the WD dipole. The noticeable effect of the negative interface modulus is the non-classical oscillations in the stress field of the WD dipole and an extra attractive image force on it. Rezazadeh-Kalehbasti et al. [111] demonstrated that the stresses are rather inhomogeneous across the NW cross section, change their signs and reach local maxima and minima far from the WD lines in the bulk or on the surface of the NW. For negative values of the surface/interface modulus and relatively small values of the ratio of the shell and core shear moduli, the surface/interface effect manifests itself through non-classical stress oscillations along the shell free surface in the case of a WD dipole and core-shell interface in both the cases of a WD dipole and an individual WD. The non-classical solution for the strain energy deviates from the classical solution with different effects caused by the surface/interface moduli on the

WD dipole and an individual WD. When the core is softer than the shell, the dipole with radial orientation of its arm has an unstable equilibrium position in the shell. In general, if the surface/interface modulus is positive, the surface/interface effects are rather weak; however, if it is negative, the effect can be very strong, especially near the shell surface.

Solution for the dipole of WDs whose lines are perpendicular to the free surfaces of the flat plate of finite thickness, is given in the works [18, 19].

Within the classical theory of elasticity, Kolesnikova et al. [112] solved a new boundary-value problem for a WD axially piercing a hollow sphere. The displacements, the stresses and the dilatation of the WD were represented in the form of series with Legendre polynomials and analyzed in detail. The related problems of WDs axially piercing a bulk elastic sphere and a spherical pore in an elastic medium were addressed as well. The authors concluded that the divergence of the WD elastic fields was eliminated everywhere in the elastic bodies with the exception of the WD line. The hollow and bulk spheres are the most screening systems for the WD in comparison with the flat layer [16] and the infinite cylinder [42] considered earlier. The distribution and the magnitude of the WD elastic fields in spherical bodies strongly depend on the presence and the size of the inner cavity. Nevertheless, the regions adjacent to the lines of positive (negative) WDs are always hydrostatically compressed (stretched), while the regions distant from these lines are always hydrostatically stretched (compressed). The formal solution for a WD axially piercing a spherical pore in an infinite elastic medium is inapplicable for analyzing the elastic fields of the WD. To get their realistic description, it is necessary to strictly take into account the boundary conditions on remote external boundaries of the body containing the WD. For example, the solution of the problem of a WD, axially piercing a sufficiently thick spherical layer, is suitable for analyzing the case of a spherical pore on the WD line.

The elastic fields found by Kolesnikova et al. [112] were used in theoretical models which described the fracture of hollow decahedral particles under chemical etching [113], the elastic strains in homogeneous [114] and core-shell [96] decahedral NPs and their relaxation through generation of CPDLs. In these models, the positive partial WD of strength $+7°20'$ lies along the axis of five-fold symmetry in a decahedral particle, which axis coincides with the line of junction of five twin domains [115]. The solution by Kolesnikova et al. [112] allowed to consider the decahedral particle as an elastic sphere (either hollow [113], or bulk [114], or composite [96]) axially pierced by the WD and to calculate the initial (unrelaxed) strain-stress states within these models.

We also mention a number of boundary-value problems solved for a circular twist disclination loop, the Frank vector of which is perpendicular to the plane of the loop. Solutions for elastic fields and energy of the twist loop in a finite thickness flat plate, near a free surface and an interface are given in the Refs. [18, 19]. In the cylinder, solid sphere and for the loop circling the spherical hole, the solutions for the twist loops can be found in the Refs. [20, 116] and [27], respectively.

5 Inclusions

The boundary-value problems for inclusions have been solved in our lab with the aim to use these solutions mainly for studying the misfit stress distribution in various composite nanostructures. Some of these results were found from more general solutions by simple limiting transitions. For example, Malyshev et al. [117] solved the problem for a dilatational inclusion in the shape of a long prism of rectangular cross section (rectangular inclusion) embedded to a thin elastic layer in such a way that the edges of the inclusion and two its faces were parallel to the layer free surfaces. Mikaelyan et al. [41] reproduced this solution and used it to analyze the model of dislocation emission from the edge of such an inclusion embedded in a free-standing nanolayer. With a limiting transition from the nanolayer to a semi-infinite medium, Gutkin et al. [99] found an explicit analytical solution for a similar inclusion in an elastic half-space and applied it to modeling the misfit stress relaxation in misfitting NWs embedded to a half space (see also Subsection 3.2).

Gutkin et al. [118–120] considered a similar rectangular inclusion with antiplane eigenstrain as a model for polytype inclusions in growing crystals of silicon carbide. With using this model, they gave a theoretical description for the elastic interaction of these inclusions with MPs (see Subsection 3.1.2) and showed that MPs must be attracted to the boundaries of the inclusion and agglomerate there with formation of elongated pores, as was revealed by their own direct experimental observations. In doing so, they solved a boundary-value problem for the rectangular inclusion interacting with the free cylindrical surface of an MP [119] and demonstrated that the equilibrium positions of MPs lie at the inclusion boundaries. Moreover, Gutkin et al. [120] found the solution for the stress field of a similar inclusion containing an elliptic pore on its boundary. The analysis of the forces exerted on MPs by the inclusion and elliptic pore showed that the pore attracts MPs until their number reaches a critical value. After that, the MPs absorbed by the pore produce a repulsion zone for new MPs, and pore growth stops. The critical pore size is determined by the values of inclusion plastic distortions. At their small values, isolated MPs form at the inclusion/matrix interface; at medium values MPs coalesce to form a pore of a certain size; at large values the pore occupies the whole inclusion boundary.

The spherical dilatational inclusion embedded in the flat finite thickness plate was considered in [20], and the related boundary-value problem was solved using MVSD.

A number of boundary-value problems have been solved for the inclusions that play the role of cores in core-shell NWs and NPs. First, infinite cylindrical inclusions with 3D dilatational eigenstrains were considered as cores in elastically homogeneous [43, 121, 122] and inhomogeneous [85] cylindrical core-shell NWs. Enzevaee et al. [56] solved a similar elastically inhomogeneous problem within the surface/interface elasticity.

Gutkin et al. [123] constructed the model of a cylindrical core with axial 1D dilatational eigenstrain and finite length in a cylindrical NW. The stress fields of this finite-length core was found through continuous distribution of virtual CPDLs with infinitesimal Burgers vectors over the side boundary of the core and integration of stress fields of these virtual CPDLs over the core length. The authors analyzed two possible ways of stress relaxation in such a composite NW – by misfit CPDLs and by mode I penny-shaped cracks. It was shown that the first way is more preferable than the second one for almost all possible real cases. The elastic solution of Gutkin et al. [123] was then used by Gutkin and Panpurin [124, 125] to study the spontaneous formation and equilibrium distribution of axial cylindrical QDs in atomically inhomogeneous pentagonal NWs.

Krasnitckii et al. solved a number of boundary-value problems for faceting cores in core-shell NWs, including the cases of axial prismatic cores of square [105, 126, 127], triangle [105, 127] and hexagonal [104, 105, 127] cross sections, and eccentric prismatic cores of rectangular [128] and trapezoidal [127] cross sections. They used these solutions for comparative analysis of critical conditions for nucleation of RPDLs (see Subsection 3.2) at the initial stages of misfit stress relaxation in such NWs [103–105, 127]. For example, Krasnitckii et al. [105] considered different sites of RPDL nucleation in the NWs with hexagonal, square and triangular shapes of the core cross section. The energy change caused by the RPDL nucleation was calculated for every case under the assumption that the shell thickness is much smaller than the core size. The corresponding critical values of the misfit parameter for the RPDL nucleation were determined and compared with each other. According to this comparison, the most favorable sites in the core-shell NWs and the optimal shapes of the RPDLs were defined. NWs with round, hexagonal, square and triangle shapes of the core cross section were ranged with respect to their stability to RPDL nucleation.

The inclusion problem for bulk spherical cores in spherical core-shell NPs was solved many years ago [129, 130] and extensively used in theoretical modeling of mechanisms of misfit stress relaxation in these systems [91, 92, 96, 131]. Gutkin et al. [93] considered the case of hollow spherical cores in spherical core-shell NPs and applied its solution to modeling of misfit CPDL generation in such NPs [92, 93]. Kolesnikova et al. [132] suggested the elastic models for finite cylindrical and truncated spherical inclusions in an infinite medium as well as for a truncated spherical inclusion in an elastic sphere [133]. As a limiting case of the latter problem, a spherical Janus particle (composed of two semispheres of different materials) was considered as well [133]. The solution for a truncated spherical dilatational inclusion in an elastic sphere [133] was also used in studying the critical conditions for the formation of misfit CPDLs in core-shell NPs with truncated spherical cores [97].

In addition, spherical two-phase inclusion in the infinite matrix as a model of the core-rim structured carbide grain in the cermet, was considered in Ref. [134].

Romanov et al. [135, 136] considered a number of boundary-value problems for flat sharp and diffusive interfaces in axially-inhomogeneous NWs. These interfaces were normal to the NW axes and separated the NWs onto cylindrical segments of different misfitting materials.

The authors presented a general solution of the isotropic elasticity problem for the sandwiched inclusion in an elastic cylinder and having axially varying eigenstrain. The technique of the solution and the results for the elastic fields and energies of dilatational inclusions with different distribution of eigenstrain, namely, constant, trapezoidal, and diffusion-like, along the axis of the cylinder, were given in full details. The technique explored the axial superpositions of infinitely thin dilatation disks inserted in the cylinder, the elastic fields of which were found in analytical form. In addition, the energies of interfaces separated domains with constant eigenstrains in the cylinder were given. It was demonstrated that the blurring of the eigenstrain in the transition region leads to a decrease in interface energy.

In the works [137, 138], a finite element method was used to calculate the elastic fields and total displacements in a surface QD and an adjusted region of the substrate. The effects of QD form factor and aspect ratio δ on QD elastic properties were analyzed. A quasilinear dependence of radial displacements on radial coordinate for spherical, elliptical, and truncated spherical QDs was demonstrated. It has been found that the displacement field does not depend on the shape and aspect ratio for QDs with $\delta > \delta_{c1}$, and the upper part of a QD remains practically undistorted for QDs with $\delta \geq \delta_{c2}$. For InSb/InAs heterosystem these critical values are $\delta_{c1} \sim 0.13$ and $\delta_{c2} \sim 0.33$. The total displacements were used for computation of TEM diffraction contrast associated with QDs [137, 138].

Along with solutions of the boundary-value problems for defects that are internal sources of elastic fields, the complete analytical solution for the plane elasticity problem of a concentrated force acting on a half-space weakened by a circular hole was found [139, 140]. The solution is based on the algorithm proposed by Jeffery [141] for elasticity problems and treated in detail by Uflyand [12] using bipolar coordinates to characterize the geometry of the problem. Earlier, this problem was solved correctly by applying numerical methods and extended to the case with an elliptical hole (see e.g., Ref. [142]. We found the biharmonic stress function describing stresses and strains in the half-space and the associated biharmonic function that allows determining the displacement field. Both functions were given in the form of Fourier series with quite compact coefficients. The stresses were written and plotted. Particular attention was paid to the displacements at the surface of the half-space. It was speculated how these displacements could be used in an inverse procedure for the identification of a circular hole diameter and position in the solid by the measurements of surface displacements induced by a concentrated force.

6 Conclusions

Thus, we have given a brief review of boundary-value problems in the theory of elasticity, which have been solved for various defects (dislocations, disclinations and inclusions) in our lab during the last three decades. We have also touched some relevant works dealing with application of the solutions found to our theoretical models describing the nucleation and development of different defect structures in the process of crystal growth and misfit stress relaxation in advanced composite nanostructures which are highly promising for use in modern electronics, optoelectronics, photonics, etc.

Based on these studies, we can conclude that theoretical description of elastic behavior of defects near inner and outer boundaries of solids within the classical theory of elasticity gives rather reliable results that in a set of cases are in good accordance with available experimental data. Although the use of more extended versions of the elasticity theory (as, for example, the strain/stress gradient elasticity and the surface/interface elasticity) looks much more attractive when dealing with nanostructures, it was demonstrated that in reality they give new important results in close vicinity (not farer than ~1 nm) of surfaces/interfaces and lines of defects.

Among the problems that seem to be of special interest in the nearest future, we can notice the following areas of research:

- boundary-value problems for defects in faceted core-shell NWs and NPs;
- boundary-value problems for inhomogeneous nanostructures with diffuse interfaces;
- theoretical models describing the elastic behavior of defects in inhomogeneous nanostructures with diffuse interfaces.

The statement and solution of the above problems will allow to get new results which are expected to better reflect the behavior of defects and related phenomena in real device nanostructures.

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