

MULTI-PARAMETER OPTIMIZATION OF LAYERED WS₂-POLYMER NANOCOMPOSITE UNDER MECHANICAL LOADING

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ABSTRACT. The aim of the study is to determine the optimal geometry and magnitude of the applied load to ensure safety and prevent delamination in a three-layered nanocomposite structure under axial mechanical loading. The structure consists of a layer of the nanomaterial tungsten disulfide (WS₂) and a substrate layer of poly(methyl methacrylate) (PMMA), which are adhesively bonded using SU-8 glue. To achieve this aim, a multi-parameter optimization problem (MOP) is formulated. It includes a two-dimensional stress function model that describes stress transfer in the considered three-layer structure. Two types of analytical solutions for the interface shear stress (ISS) are derived, featuring real and complex roots. The decision variables in MOP include the external load, layer thicknesses, and structure length. The optimization criterion is defined as the minimization of the difference between the model ISS and ultimate shear stress (USS) in the adhesive layer to assure no delamination occurs in the nanocomposite structure. A genetic algorithm and alternative optimization approach developed within the framework of “Mathematica” are implemented for the optimization of both model solutions. As a result, optimal values for the given external load, layer thicknesses, and structure length are obtained for considered nanostructure. For the case of an ISS model solution with real roots, the optimization procedures ensure optimal geometries that physically correspond to thinner structural layers, but they are limited at lower possible loads. In contrast, for the case of a model solution for the ISS with complex roots, solutions for the optimal geometries of the nanostructures were obtained with thicker layers requiring higher loads, than thinner ones, but delamination does not occur.

KEYWORDS: 2D stress function model, interface shear stress, genetic algorithm, multi-parameter optimization problem, geometry parameters, external load, WS₂/SU-8/PMMA nanocomposites, static mechanical loading.

1. INTRODUCTION

One of the significant representatives of the family of TMDs from the point of view of properties and applications is tungsten disulfide (WS₂). It consists of three atomic layers of W layers sandwiched between two S layers, which enable its Young’s modulus to be 236 ± 65 GPa that is comparable to that of steel [1]. It has an indirect band gap of ~ 1.9 eV and unique chemical properties, that define its wide area of application as production of strain-engineered devices such as transistors [2], photo-detectors [3], photovoltaic devices [4] as well as in the production of multifunctional polymer nanocomposites [5]. On the other side, incorporating WS₂ nanoparticles or nanosheets into polymer matrices can enhance the mechanical, thermal, and electrical properties of the resulting nanocomposites. Applying different strain techniques such as mechanical stretching, bending or

applying external pressure to WS₂ can induce strain in the material, changing its electronic, optical and mechanical properties [6]. Therefore, understanding how different types and levels of strain affect WS₂ is vital to tailoring its properties to specific applications. Falin et al. (2021) [7] applied finite element (FE) analysis and density functional theory (DFT) to determine the effects of in-plane strain and out-of-plane compression on the sliding energies in high-quality atomically thin tungsten dichalcogenides produced by mechanical exfoliation. Wang et al. (2020) [8] combined both PL spectroscopy and Raman spectroscopy to monitor the strain distribution and stress transfer of monolayer WS₂ on a flexible polymer substrate and also in thin film bulk nanocomposites. Tang et al. (2021) [9] investigated the influence of different defect types, defect density, and different ambient temperatures on the mechanical properties (i.e., Young’s modulus and crit-

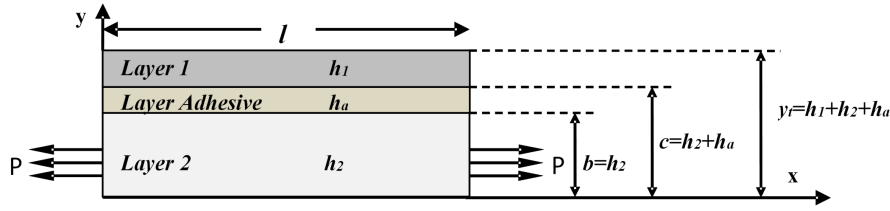


FIGURE 1. Representative volume element (RVE) of 3-layer $WS_2/SU-8/PMMA$ nanocomposite structure, where: h_1 – nanomaterial layer (WS_2); h_a – adhesion layer ($SU-8$); h_2 – substrate layer ($PMMA$), P – static tension force.

ical stress) of WS_2 under different strains using the multiscale simulation, DFT, MD analysis, and FE.

Optimizing the geometry and loads in TMDs-based nanocomposites is crucial for enhancing stress control and unlocking their full potential across various applications including flexible electronics and structural materials, where superior strength, efficiency, performance, reliability, and durability are paramount. Moreover, it is crucial to identify the safe operating zones of the structures under consideration, particularly when they are subjected to complex loadings. Tserpes and Koumpias, (2015) [10] proposed a numerical methodology combining the ANSYS FE code and a progressive damage modeling module for optimizing the geometry of composite structures with regard to strength by maintaining the initial weight. The methodology has been applied for H-shaped adhesively bonded joints subjected to quasi-static load. Motlagh et al. (2023) [11] proposed a framework based on genetic algorithm for optimizing energy harvesting from laminated composite panels integrated with (multiple) piezoelectric patches. Anh (2023) [12] applied a differential evolution optimization algorithm combined with Galerkin method for investigation of the effect of elastic foundations, geometrical parameters and initial imperfection on the natural frequency in an imperfect nanocomposite multilayer organic solar cell.

It is noteworthy that there are not many studies in the literature related to the development of optimization approaches specifically tailored to the geometry of TMDs (transition metal dichalcogenides)-based polymer nanocomposites. While optimization methods from the field of metaheuristics have been applied to composite materials constructed from various layers of metal compounds, it appears that similar approaches haven't been extensively explored for TMDs-based polymer nanocomposites.

This study proposes a multi-parameter optimization approach to determine the optimal geometry and magnitude of the applied load for ensuring safety and preventing delamination in a three-layered adhesively bonded tungsten disulfide/poly(methyl methacrylate) ($WS_2/PMMA$) nanocomposite structure under axial mechanical loading. The optimization framework employs a two-dimensional stress function model to describe stress transfer within the $SU-8$ in three-layer structure. It involves five decision variables, including the external load, the thickness of each layer, and

the structure length. The objective function aims to minimize the difference between model interface shear stress and its critical value at which delamination occurs, to assure no delamination occurs in the nanocomposite structure. The multi-parameter optimization problem was solved using two optimization algorithms, one of which is the genetic algorithm. Implementation of these algorithms yielded optimal values for the decision parameters, ensuring safety and preventing delamination in the considered nanocomposite structure.

2. 2-D STRESS-FUNCTION MATHEMATICAL MODEL

In this section, a 2D analytical model (variational stress-function method) for stress fields in 3-layer nanocomposites subjected to mechanical loading is presented in a concise form (Figure 1, for details see [13]).

The proposed method allows the analytical solution of a fourth-order ordinary differential inhomogeneous equation with constant coefficients, concerning the unknown axial stress function σ_1 in the first layer (WS_2). Two types of analytical solutions (Eqs. (1) and (2)) for the axial stress σ_1 in the first layer are derived, wherein the coefficients depend on the geometry of the three-layer nanocomposite, its material properties, and external loading.

$$\sigma_1(x) = C_1 \cdot \exp(\lambda_1 \cdot x) + C_2 \cdot \exp(\lambda_2 \cdot x) + C_3 \cdot \exp(\lambda_3 \cdot x) + C_4 \cdot \exp(\lambda_4 \cdot x) - A \quad (1)$$

$$\sigma_1(x) = \exp(-\alpha x) [M_1 \cos(\beta x) + M_2 \sin(\beta x)] + \exp(+\alpha x) [M_3 \cos(\beta x) + M_4 \sin(\beta x)] - A \quad (2)$$

In Eqs. (1) and (2), the constant A represents the solution for inhomogeneous ordinary differential equation and is dependent on the external static load ($\sigma_0 = P/h_2$), while C_i and M_i are the integration constants in the model solutions, determined by the corresponding boundary conditions [13]. All other stresses, including the ISS, are expressed by Eqs. (1) and (2) and their derivatives. Eq. (2) represents the solution for case of four complex roots $\pm(\alpha \pm i\beta)$, whereas Eq. (1) corresponds to the scenario of four real roots λ_i . The nature of the roots depends on the

| Model solution | σ_0 [Pa] | l [m] | h_1 [m] | h_a [m] | h_2 [m] |
|----------------|-------------------------------------|--|--|--|--|
| Eq. 1 | $1 \cdot 10^5 \div 1 \cdot 10^7$ | $1 \cdot 10^{-5} \div 1 \cdot 10^{-4}$ | $0.6 \cdot 10^{-9} \div 8 \cdot 10^{-9}$ | $1 \cdot 10^{-9} \div 1 \cdot 10^{-7}$ | $1 \cdot 10^{-7} \div 1 \cdot 10^{-3}$ |
| Eq. 2 | $1 \cdot 10^5 \div 1 \cdot 10^{10}$ | $1 \cdot 10^{-5} \div 1 \cdot 10^{-4}$ | $0.6 \cdot 10^{-9} \div 5 \cdot 10^{-9}$ | $1 \cdot 10^{-9} \div 1 \cdot 10^{-7}$ | $1 \cdot 10^{-7} \div 1 \cdot 10^{-3}$ |

TABLE 1. Lower and upper boundaries for varying the decision variables.

chosen layers' thicknesses and length of the nanocomposite structure [14].

The model criterion for no interface delamination in the nanostructure, where USS represents the ultimate shear stress of the interface (adhesive) layer, is as follows:

$$ISS = \sigma_{xy}^{(a)}(x) = h_1 \sigma_1' \leq \sigma_{USS}^{(a)}. \quad (3)$$

If exists, graphically delamination initiates at both ends of the structure, representing the intersection of the ISS model curve with the straight horizontal line corresponding to the USS.

3. MULTI-PARAMETER OPTIMIZATION PROBLEMS FORMULATION

To investigate the influence of the geometry of the considered WS₂/SU-8/PMMA nanocomposite structure and the applied load on the delamination, multi-parameter optimization problems are formulated and solved for the two types of ISS model solutions, featuring real and complex roots. These formulations define the relevant decision variables, constraints, and objective functions.

3.1. DECISION VARIABLES

All geometric characteristics of the considered nanostructure, including layer thicknesses (h_1 , h_a , h_2) and the length of the structure (l), as well as the external load (σ_0), affect delamination. That's why all these factors are chosen as decision variables.

3.2. CONSTRAINTS

The MOP includes constraints on the bounds of variation of the decision variables, as well as a constraint that tracks whether the ISS reaches the USS (Eq. (3)).

3.3. OBJECTIVE FUNCTION

The aim of the optimization for both types of model solutions for ISS, with real and complex roots, is to find the optimal values of all 5 decision variables at which the minimal difference between ISS and USS is obtained. With the latter in mind, the objective function represents the minimization of the difference between ISS and USS (Eq. (3)).

4. OPTIMIZATION METHODS

For solution of formulated MOPs with the both types of analytical solutions for ISS with real and complex roots, two approaches have been applied. The first one

calls BASIC genetic algorithm (GA) [15] and the second represents an optimization procedure developed by "Wolfram Mathematica 13.0.1" software.

BASIC GA operates on foundational principles common to all genetic algorithms. It includes various types of schemes for the genetic operators for selection, crossover, and mutation, providing users with the flexibility to choose among them to address a specific optimization problem. Additionally, it can be adjusted for the concrete problem by tuning its global and local parameters. The first ones are: the number of generations (iterations); the number of samples selected for the process of recombination (crossover), the probabilities for crossover and mutation. The local parameters are related with the different schemes of the genetic operators.

The other optimization method represents a procedure developed using the software package "Mathematica". In this procedure, different sets of geometry are included in the optimization loop for the interval of values for external load, checking whether the objective function (Eq. (3)) is satisfied or not at the current geometry parameter values. It iterates as many times as the user needs until near-optimal solutions are reached, e.g, to ensure, that delamination does not occur.

For the considered nanocomposite structure WS₂/SU-8/PMMA, the aim is to simultaneously determine the optimal values of the decision variables (length, layer thicknesses h_1 , h_a , h_2 , and external load σ_0), at which the objective function has the minimum value. The decision variables vary within predefined technological boundaries. The formulated multi-parameter optimization problem is solved using BASIC GA approach under various combinations of genetic operator schemes for selection, crossover, and mutation and different sizes of populations and sampling pools as well as different number of generations. The latter is the used as termination criterion.

5. RESULTS AND DISCUSSION

The material properties, Young's modulus E (Pa), and Poisson's ratio ν (-) of the considered nanocomposite structure (Figure 1) WS₂/SU-8/PMMA are taken from [8] as follows: $E(\text{WS}_2) = 270$ GPa, $E(\text{SU-8}) = 2$ GPa, $E(\text{PMMA}) = 3.5$ GPa, $\nu(\text{WS}_2) = 0.22$, $\nu(\text{SU-8}) = 0.22$, $\nu(\text{PMMA}) = 0.35$. In addition, the lower and upper boundaries of all 5 decision variables have been defined (Table 1). The adhesive (interface) is a SU-8 glue with USS = 30 MPa. It should be borne in mind that the adhesive properties, especially the critical

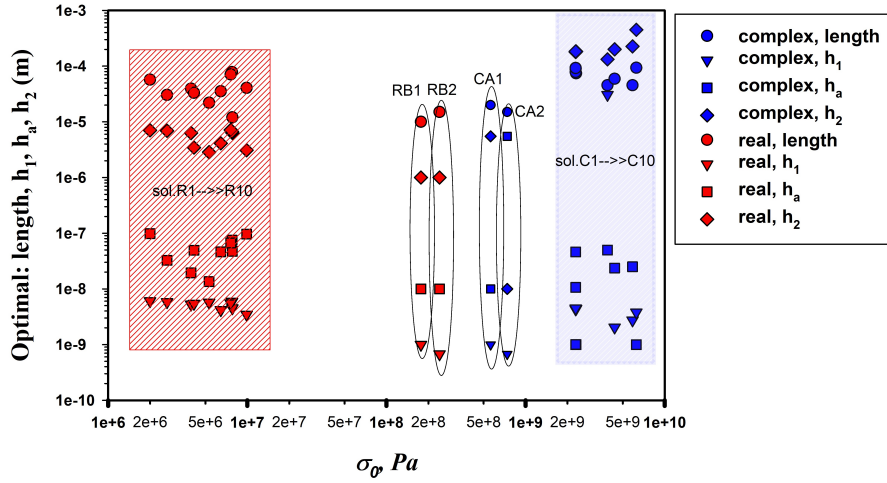


FIGURE 2. Optimal solutions for 5 decision variables from BASIC GA and Mathematica optimization algorithms: complex (blue) and real roots (red).

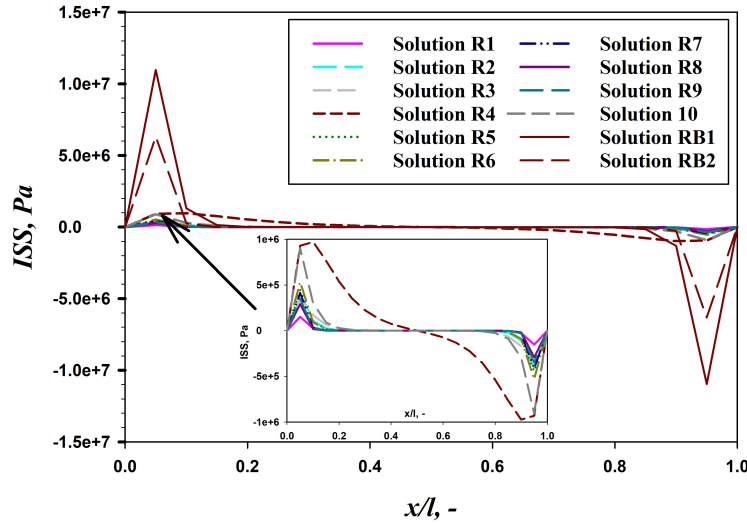


FIGURE 3. Model interface shear stress solutions obtained at the optimal values of decision variables. Case of model solution with real roots.

value of interfacial shear stress, play an important role in the delamination of nanostructures.

The main purpose of the study is to conduct an optimization of the geometry and the external load of the considered nanostructure, specifically to identify the optimal values of the decision variables at which the objective function reaches its minimum value. To achieve this goal, the MOPs for the both ISS model solutions formulated in the previous section are defined. These problems were solved using BASIC GA and the optimization procedure developed in Mathematica.

In Figure 2, the optimal values of the decision variables (external load, layer thicknesses, and the length of the overlap zone) for the cases of complex and real roots models solutions are plotted (symbolically).

It can be seen from the Figure 2 that along the ordinate, each decision variable changes within certain boundaries (intervals) for each of the two types of solutions (1) and (2) for ISS included in Eq. (3). The

boundaries of the changes in the optimal thicknesses of PMMA (h_2) and the interface layer (h_a) for the cases of real and complex roots are particularly well distinguished. The intervals of variation for h_1 and l are almost similar for both possible solutions (Eq. (1)) and (Eq. (2)). Along the abscissa, each different set of geometry data corresponds to a particular mechanical load. Thus, for each combination of the five decision variables, the objective function is satisfied, or the predicted ISS model at those load values and geometry is equal to or below the USS value. Figures 3 and 4 present part of the ISS distributions along the length of the nanocomposite obtained at optimal values of the decision variables. It can be seen that for each type of solution, the optimal values of the decision variables satisfy the objective function in the considered nanocomposite structure. In the case of ISS calculated for real roots (Eq. (1), Figure 3), it is notable that the solutions obtained with the BASIC GA (marked

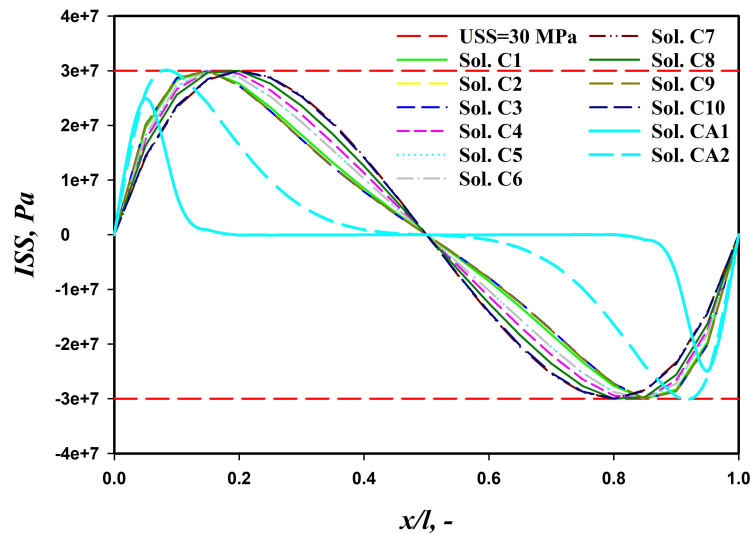


FIGURE 4. Model interface shear stress solutions obtained at the optimal values of decision variables. Case of model solution with complex roots.

with numbers R7, R8, R9, and R10) for the geometry of the considered nanostructure and loads ensure an absolutely safe operation of the structure (far from USS). These solutions provide a significant difference between ISS and USS, with no observed delamination of the structure. Conversely, solutions obtained with the other optimization procedure (marked as Sol RB1 and Sol RB2) provide geometry and mechanical loading where ISS is closer to USS, but still do not reach it. Figure 4 shows solutions for the ISS calculated with complex roots. The majority of these solutions are obtained using BASIC GA (marked with numbers C1 to C10), while the remaining solutions are derived from another optimization procedure (marked as Sol CA1 and Sol CA2). It can be seen from Figure 4 that for the most of solutions, a minimum difference between ISS and USS is reached. For sol. CA1 this difference is greater, but still fulfilled the criterion Eq. (3).

6. CONCLUSIONS

This study proposes an optimization framework aimed at determining the geometric parameters and applied load magnitude necessary to ensure the safe operation of a three-layer adhesively bonded WS₂/SU-8/poly(methyl methacrylate) nanocomposite structure under axial mechanical loading. The optimization framework incorporates a two-dimensional stress function model that characterizes stress transfer within the three-layer structure. Two types of model analytical solutions for the ISS are derived for two cases with real and complex roots and a model criterion, based on ISS is included in the optimization framework. As decision variables, the external load, layer thicknesses, and structure length are considered, varying within predefined technological boundaries. The objective function aims to minimize the difference between ISS and USS in the model criterion. Two optimization

approaches were applied for both types of model solutions (with real and complex roots) – BASIC GA and an optimization procedure developed with software “Mathematica”. These methods have yielded optimal results for the geometry and loading of the structure in question, ensuring the absence of delamination. The obtained sets of 5 optimal values can be divided into two classes, depending on the used model solutions for ISS. Physically, the sets for real roots correspond to thinner structures and, accordingly, to lower loads, and vice versa – thicker structures and larger loads at complex roots. Regardless of the type of solutions, the criterion of no delamination in the considered structure is satisfied which is validated by ISS distributions calculated at optimal values found. From the safety point of view, a thinner design of considered nanocomposite structure is preferable, but at limited loads. Thicker ones will require higher loads, than thinner ones, but delamination does not occur.

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