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PARAMETRIC ANALYSIS FOR INTERPHASE SHEAR STRESS IN MOS_2/PET NANOCOMPOSITE UNDER THERMO-MECHANICAL LOADING

Rayka Vladova[a,*], Tatyana Petrova[a], Elisaveta Kirilova[a], Boyan Boyadjiev[a], Apostol Apostolov[a], Wilfried Becker[b], Alexsander Moravski[c]

[a] *Bulgarian Academy of Sciences, Institute of Chemical Engineering, Acad. G. Bonchev str., Bl.103, 1113 Sofia, Bulgaria*

[b] *Technical University – Darmstadt, Institute of Structural Mechanics, Franziska-Braun-Str. 7, L5/01 347a, 64287 Darmstadt, Germany*

[c] *Sofia University St. Kliment Ohridski, Faculty of Mathematics and Informatics, James Bourchier Blvd. 5, 1164 Sofia, Bulgaria*

[*] corresponding author: r.vladova@iche.bas.bg

Abstract. In this study, a parametric analysis on the factors, that influence the value of theoretical interphase shear stress (ISS) in nanocomposite MoS_2/PET, subjected to thermo-mechanical loading has been performed. The theoretical value of ISS is calculated based on obtained analytical solutions for the interfacial shear stress. The sensitivity of following parameters on the ISS in the considered nanostructure is investigated: the thicknesses of the nanocomposite layers, the length of the nanocomposite, the magnitude of the applied mechanical load, the applied temperature difference. It is found that the interface thickness does not affect the ISS value. The magnitude of the applied mechanical load has a strong influence on the magnitude of the ISS. The temperature difference (pure thermal loading) also affects the ISS value, but to a lesser extent. It should be noted, that in the case of combined loading (thermo-mechanical) the overall effect is additive. The thicknesses of MoS_2 and PET mostly affect ISS, especially the substrate thickness. The obtained results are graphically illustrated and can be used for the fast prediction of ISS in micro scale in similar nanocomposite devices or parts thereof such as sensors, nano- and optical electronic devices, energy devices, etc.

Keywords: Molybdenum disulfide (MoS_2), parametric analysis, interphase shear stress, nanocomposite, thermo-mechanical loading.

1. Introduction

In recent years, there has been an increased interest in nanocomposite materials, which is indicated by the high publication activity in the global databases Web of Science and Scopus. A large part of the research is focused on the development of new polymer composites and the study of synthesis methods. One of the widespread 2D materials is molybdenum disulfide (MoS_2) due to its mechanical properties and numerous applications [1]. Significantly lower is the share of research regarding analytical methods for stress/strain modeling in nanocomposite structures. Considering the increasingly wide application of nanocomposites in industry, it is of particular importance to investigate the specific loads and design of nanocomposite structures. One of the most important characteristics for stress transfer efficiency in nanocomposites, subjected to mechanical or thermo-mechanical loading, is the value of interphase shear stress τ (or strength), which arises at the interphase between nanomaterial and polymer substrate. Du et al. 2022 [2] determine the strain field of MoS_2 and the tangential intermediate shear stress (ISS) distribution during the substrate stretching process. The research presents a method for determining the surface properties of Graphene/MoS_2 heterostructures in which the stress field of the upper Graphene and the lower MoS_2 structure is determined. Typically, the ISS value is obtained based on data from strain measurements using Raman and photoluminescence (PL) spectroscopy or with other methods, and then using the relation between ISS and strains (from continuum mechanics or shear-lag model). Dong et al. [3] use (PL) spectroscopy to study interfacial voltage transfer from a polymer substrate to mono- and multilayer molybdenum disulfide (MoS_2) under stress. The study determined the shear strength limit for various combinations of 2D nanomaterials and polymer substrates by performing stress mapping at various stress levels. It is found that the stress transfer length increases with increasing number of layers and there is no significant change for mono and bilayer MoS_2. It is essential to investigate the mechanical and physical properties of heterostructures. A study of the mechanical properties of multilayer MoS_2 and a graphene/MoS_2 heterostructure were made by [4] by molecular dynamics simulation under uniaxial tensile stress and normal compression. The study shows that the stiffness of the heterostructure is significantly greater than MoS_2, which is due to the higher elastic constants of graphene.

To bridge the gap between theory and experimental data, the focus of the present work is on the influence of 4 geometrical and 2 loading parameters on interfacial shear stress in nanocomposite structure MoS_2/Interphase/polymer nanocomposite, subjected to thermo-mechanical loading. In this study, a parametric analysis (PA) is performed in order to determine the influence of geometry (thicknesses of nanocomposite layers and length of the structure) and loading (mechanical and thermo-mechanical) on the delamination in the nanocomposite structure MoS_2/PET. According to our previous works [5, 6], two analytical model solutions for ISS are used in PA for the considered nanostructure, as well as the model criteria for delamination. The critical values of the geometric parameters and loading are obtained after which delamination in the structure appears. The proposed method of PA as well as the model solutions and criteria, could be successfully applied to the similar three-layer nanocomposites if the model assumptions are fulfilled (see for details [6]).

2. Materials and methods

The study used 2D analytical modeling of stress fields in 3-layer nanocomposites subjected to thermomechanical loading (Figure 1); the model is validated in our previous works [5–7] for similar structures. The applied method makes it possible to solve an analytical ordinary differential inhomogeneous equation of the 4^{th} order with constant coefficients, with respect to the unknown axial stress function σ_1 in the first layer (nanolayer) [6, 7]. All other stresses in the layers, including the interphase shear stress are expressed by σ_1 and its derivatives. Here, only the most important formulas including two types of derived analytical model solutions for the axial stress σ_1 in the nanolayer (Eq. (1) and (2)) are presented, with coefficients depending on the geometry of the three-layer nanocomposite, its material properties and external load:

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

$$\sigma_1(x) = \exp(-\alpha x)\left[M_1 \cos(\beta x) + M_2 \sin(\beta x)\right] + \exp(\alpha x)\left[M_3 \cos(\beta x) + M_4 \sin(\beta x)\right] - A \tag{2}$$

In Eq. (1) and (2) the constant A is the solution for non-homogeneous ODE and depends on external static load and temperature difference, applied to whole structure and C_i and M_i are the integration constants in the model solutions, determined from the respective boundary conditions [5]. The value of ISS

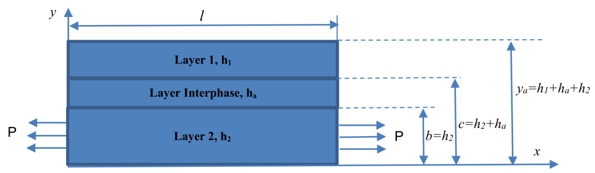


Figure 1. Scheme of the three layer nanocomposite structure, where: h_1 – nanomaterial layer; h_a – interphase layer; h_2 – substrate layer, P – static tension force [N.m] and $\sigma_0 = P/h_2$.

is calculated by $\sigma_{xy}^{(a)}(x) = h_1 \sigma_1'(x)$, where in the right hand side Eq. (1) or (2) are used, respectively.

In this work, both solutions are considered in PA; Eq. (2) corresponds to the case of 4 complex roots $\pm(\alpha \pm i\beta)$, while Eq. (1) corresponds to the case of 4 real roots λ_i [7]. For convenience, the following notations will be used in the text below for the type of solution used in the calculation of ISS in the PA: Case 1 for real roots and Case 2 for complex roots. It is worth to note [5], that the type of roots (and solutions for ISS, respectively) depends on the chosen geometry of the nanocomposite structure (layers' thicknesses and its length). For the considered nanostructure MoS_2/PET the middle layer (Figure 1) is an interphase layer between MoS_2 and PET, with thickness h_a. The interphase (adhesive) layer is modelled according to the Zhu and Narh approach [8]. Material properties, geometry, loading and coefficients of thermal expansion (CTE) for all layers are given in Table 1.

The model criterion for the interphase delamination in the considered structure is defined, where USS is the ultimate shear stress of interphase layer:

$$\sigma_{xy}^{(a)}(x) = h_1 \sigma_1' \geq \sigma_{USS}^{(a)} \tag{3}$$

Graphically, the delamination starts from both ends of the structure and represents the intersection of the ISS model curve with the straight horizontal line corresponding to the USS [3].

3. Results of parametric analysis of molybdenum disulfide/Interphase/PET nanocomposite

The PA of the factors, influencing interphase delamination, was performed and investigated for Case 1 and Case 2 of combined loaded MoS_2/Interphase/PET nanocomposite (Table 1). The factors taken into account in PA are: influence of mechanical load σ_0 on ISS, layers' thicknesses h_1, h_a, h_2, layers' length l and influence of temperature load ΔT. The USS value is 0.26 MPa, taken from [3]. All material properties and fixed values for geometry, loading and other data during the PA for Case 1 and Case 2 of considered nanocomposite are presented in Table 1. The values of coefficients of thermal expansion for MoS_2 and PET

Case studies	**Young's modulus [GPa]**			**Poisson ratio [–]**			h_1 **[nm]**	h_a **[m]**	h_2 **[m]**	l **[µm]**	σ_0 **[Mpa]**
For ISS calculation	MoS_2	**Inter-phase**	**PET**	MoS_2	**Inter-phase**	**PET**	MoS_2	**Inter-phase**	**PET**	**All layers**	
Case 1 (real roots)	270	11.5	2.3	0.25	0.34	0.43	0.65	3e-08	9e-07	72	15
Case 2 (complex roots)	270	3	2.3	0.25	0.34	0.43	0.65	2e-09	5e-05	72	25

TABLE 1. Material properties, geometry and mechanical load for MoS_2/Interphase/PET nanocomposite.

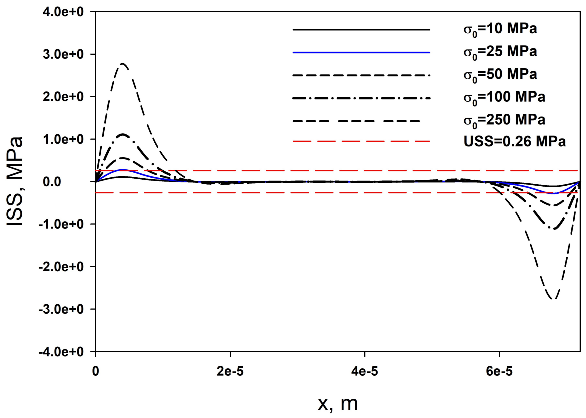


FIGURE 2. Influence of the magnitude σ_0 of mechanical load on the ISS, for considered MoS_2/interface/PET, for complex roots.

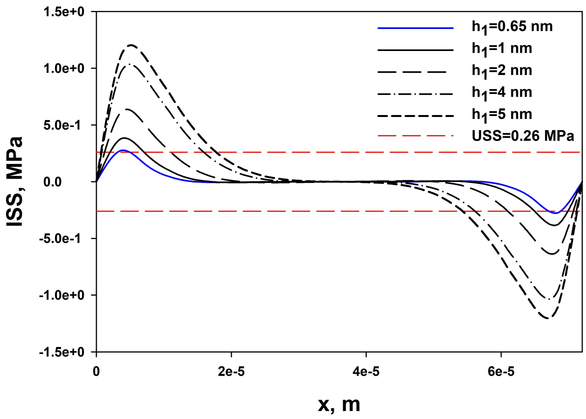


FIGURE 3. Influence of the thickness h_1 on the ISS, for MoS_2/Interface/PET for complex roots.

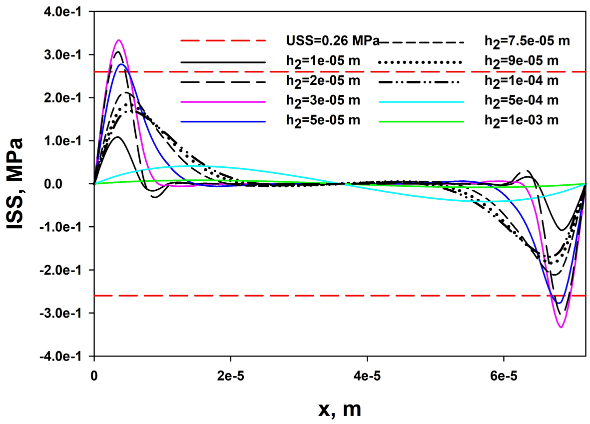


FIGURE 4. Influence of the thickness h_2 on the ISS, for MoS_2/Interface/PET for complex roots.

are 5e-06 [1/K] and 5.96e-06 [1/K], respectively. In case of thermo-mechanical loading of nanocomposite ΔT varies between 0 (pure mechanical loading) and 500 K [7]. All calculations and corresponding parametric analysis were done in Mathcad environment.

3.1. PA FOR CASE 2

The influence of mechanical load σ_0 on the ISS, Case 2 is depicted on the Figure 2. The figure shows that over 25 MPa external mechanical load at a fixed geometry for Case 2 (Table 1) of the considered MoS_2/interphase/PET nanocomposite structure, delamination is observed.

Regarding the influence of h_1 on ISS, Case 2, it is depicted on the Figure 3. It is seen, that increasing the thickness above that of the MoS_2 monolayer (0.65 nm) the delamination arises, i.g, the monolayer thickness is a critical value. These results are in agreement with results of Dong et al. [3] for MoS_2/PMMA, that "monolayer MoS_2 is more effective in terms of interfacial stress transfer compared to multilayer one".

Figure 4 portrays the influence of h_2 on ISS, Case 2. If PET thickness $h_2 > 50$ µm, the delamination is not appearing. Influence of h_a is negligible, ISS does not depend on h_a and it is not presented here. The impact of the length l on the ISS, Case 2 is seen up to 90 µm; after $l > 90$ µm – at fixed layers' thicknesses and load (Table 1), the delamination not arises. The maximal value of ISS is reached at about $l = 15$ µm as is clearly seen in Figure 5.

The effect of thermal loading is depicting on the Figure 6. If a sufficient cooling temperature difference ($\Delta T = -100$ K or more) is applied to the mechanical loading where we have already established delamination, as a result the deboning is no longer observed in the considered structure. This is probably due to the differences in CTEs of MoS_2 and PET and resulting additional compressive strains occurring after an applied thermal load; all this ultimately reduces the ISS value below the critical one. In contrast, the opposite situation has place (the positive temperature

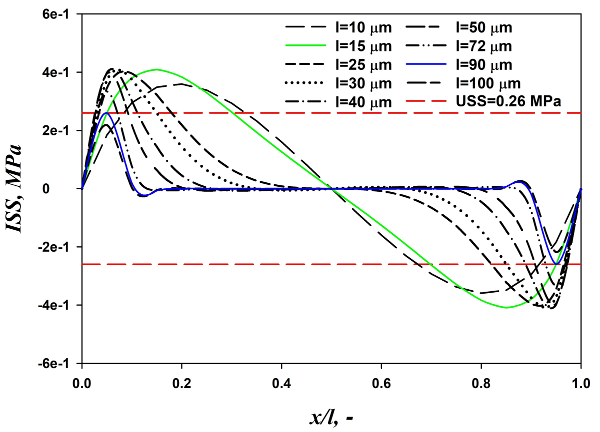


Figure 5. Influence of length on the ISS, for MoS_2/Interface/PET for complex roots.

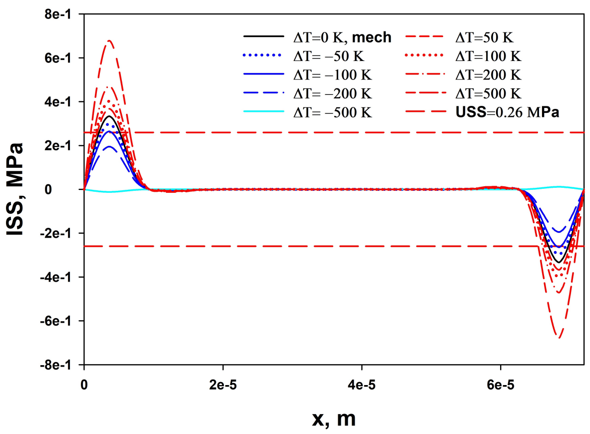


Figure 6. Influence of temperature load on the ISS, for MoS_2/Interface/PET for complex roots.

difference increased already observed delamination) in the case of heating, applied to the mechanically loaded nanostructure.

3.2. PA for Case 1

Before presenting the results from PA for ISS Case 1, it should be noted, that during the calculations we found that solution for ISS Case 1 in the considered nanostructure exists at very thin intervals for parameters h_a and h_2. The used model [5–7] allows more than one solution if the geometry of the structure is appropriately chosen. Physically, the Case 1 corresponds to thinner nanocomposite, and Case 2 to thicker one.

The influence of mechanical load σ_0 on the ISS Case 1, is shown in Figure 7. At a fixed geometry of the considered MoS_2/interphase/PET nanocomposite structure, delamination is not observed for applied loads.

The influence of h_1 on ISS Case 1, is depicted on the Figure 8. The figure shows, that keeping MoS_2 thickness $h_1 < 2.66$ nm, at fixed other parameters, the delamination is not appearing; over this value it appeared. For comparison, on Figure 3 the critical

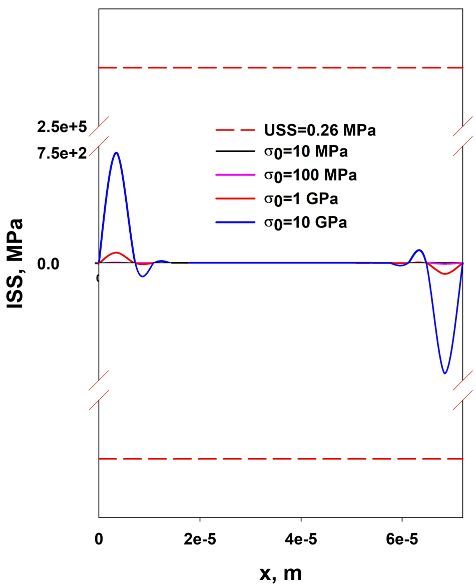


Figure 7. Influence of the magnitude σ_0 of mechanical load on the ISS, for considered MoS_2/Interface/PET at real roots.

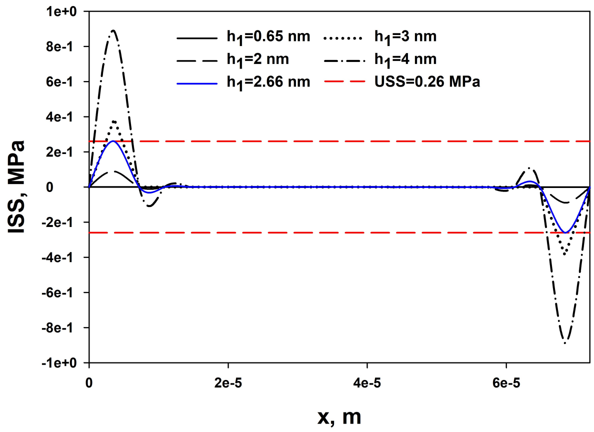


Figure 8. Influence of the thickness h_1 on the ISS, for MoS_2/Interface/PET at real roots.

value for h_1 Case 2, after which delamination arises, is 0.65 nm, here, in Figure 8 for Case 1 it is 2.66 nm, which confirm the fact that thicker layers are more stable against delamination. The influence of h_a on ISS is negligible and is not represented here.

Figure 9 portrays the influence of h_2 on ISS Case 1. Keeping PET thickness h_2 in the range of 0.81 μm ÷ 1.2 μm, the delamination is not appearing. It should be noted, that existence of positive roots and, the existence of model solutions for axial stress and ISS, respectively, are inextricably bound up with very thin interval for h_2.

Figure 10 presents the influence of length l on the ISS: after l >38.25 μm at fixed other layers' thicknesses, the delamination does not occur.

The effect of thermal loading is determined: for higher lengths of structure layers, at 72 μm and more, the influence of ΔT on ISS is negligible, as seen in

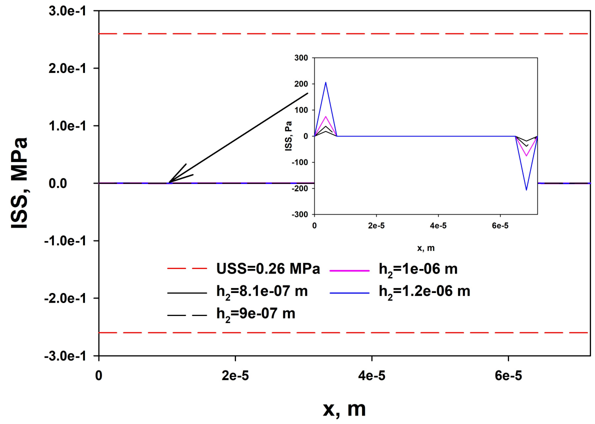


Figure 9. Influence of the thickness h_2 on the ISS, for MoS_2/Interface/PET for real roots.

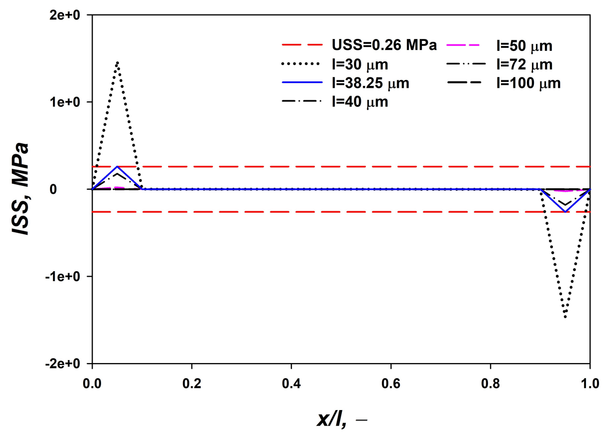
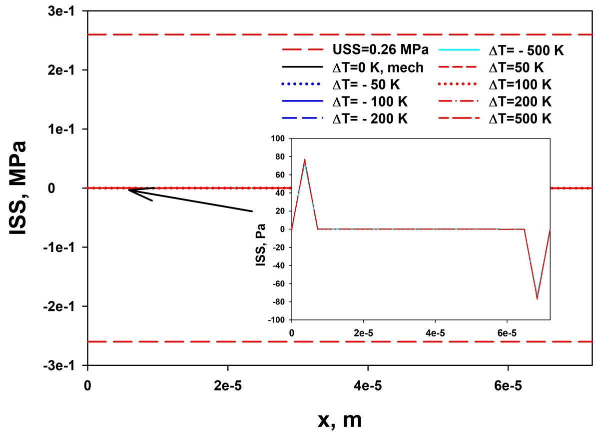
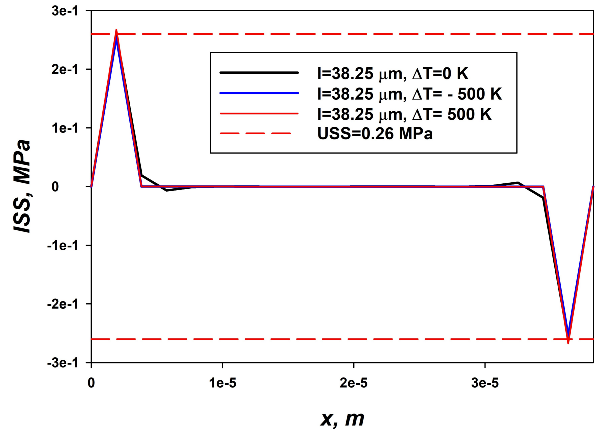


Figure 10. Influence of length on the ISS, for MoS_2/Interface/PET for real roots.



(a). At fixed length 72 µm.



(b). At 38.25 µm.

Figure 11. Influence of temperature load on the ISS, for MoS_2/Interface/PET for real roots.

Figure 11a. If a sufficient cooling temperature difference (ΔT = - 500 K) is added to the mechanical loading, at fixed length 38.25 µm (i.e. where we have already established onset of delamination), debonding is no longer observed in the considered structure (Figure 11b).

4. Conclusions

In this study, the influence of the mechanical and thermal load, the thicknesses h_1, h_2, h_a, as well as the influence of the structure length on the theoretically predicted values of ISS in thermo-mechanically loaded 3-layer nanocomposite structure MoS_2/Interphase/PET is shown, by parametric analysis. The model values of ISS are used, based on the analytical solutions for ISS at two cases with different nanocomposite structure geometry (Case 1 and Case 2) [6, 7]. As a criterion for influence of these 6 parameters on ISS, the model non-linear condition for delamination in the structure is used, i.e., it requires that model ISS is greater than USS in the middle interphase layer. Received results allow determining the significance of the factors affecting the delamination in the investigated molybdenum disulfide/polymer nanocomposite structure at two distinct cases of its geometry.

It is found that the interphase thickness does not affect the ISS value for both cases. The magnitude of the applied mechanical load has a strong influence on the magnitude of the ISS for both cases. The temperature difference also affects the ISS value for Case 2, but to a lesser extent and has an additive effect for heating when the delamination already exists as a result of applied mechanical load. In the case of cooling, the effect could be opposite. The thicknesses of MoS_2 and PET mostly influence model ISS for both Cases 1 and 2, especially the substrate thickness. The effect of length on ISS is more pronounced for both cases for ISS at short lengths of the nanostructure. The obtained results are graphically illustrated and can be used for fast prediction of ISS in micro scale in similar nanocomposite devices or parts thereof such as sensors, nano- and optical electronic devices, energy devices, etc.

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