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Numerical evaluation of the strength of graphene-reinforced metal matrix composites

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Abstract. This work evaluates the overall strength of graphene-reinforced metal matrix composites employing a computational homogenization procedure. The simulations are carried out using the finite element method and are based on unit cells representing an aggregate composed of a metallic matrix, obeying the von Mises criterion, which is reinforced with high strength and stiff plane inclusions mimicking graphene. Uniaxial displacement boundary conditions are imposed. The macroscopic stress components are calculated from the reaction force obtained from the simulations and assumed to be the mean stress component in that direction after reaching an asymptotic response. The study considers different volume fractions and orientations of the reinforcement, thus addressing the effects of such material features on the macroscopic yield behavior.

Keywords: Metal matrix composites, Graphene-reinforcement, Plasticity, Computational homogenization, Finite element method

1 Introduction

The concept of composite materials allows combining physical properties of different materials, resulting in an aggregate with the desired characteristics (Novoselov et al. [1], Stankovich et al. [2]). This increasingly broad technology in the development of more efficient materials and structures. Process advancement of innovation opportunities - such as a range of additive manufacturing (AM) opportunities - has a range of additive innovation opportunities. Considering the metallic matrix composite materials (MMC), there are studies demonstrating that the addition of carbon nanostructures is a promising strategy for the reinforcement of MMCs, without a significant increase in swight (Shin et al. [3], Chen et al. [4]).

With the production of reinforced MMCs, it would be possible to produce lighter structures, ideal for the automotive and aerospace industries. Faced with the difficulties addressed in molding and machining processes, MA is an alternative for the production of MMCs. However, given that this topic is still an emerging issue, investigations related to the understanding, characterization and modeling of the mechanical behavior of printed materials are essential for their safe application in mechanically responsible structures (Yin et al. [5]). Given this need, this project proposes to investigate the influence of graphene addition on the elastic-plastic behavior of MMCs produced by additive manufacturing. At this point, the investigation will take place in the numerical fields.

The morphology, distribution and orientation of the reinforcement nanostructures will depend on processing conditions. Which will influence the properties and performance of the resulting materials (Huang et al. [6], Neubauer et al. [7], Zhang et al. [8]). Bearing in mind the aspects discussed above, the main objective of the present proposal is to investigate and model the combined effects of the volumetric fraction and orientation of graphene reinforcements on the elastic-plastic behavior of metal matrix composites.

2 Methodology

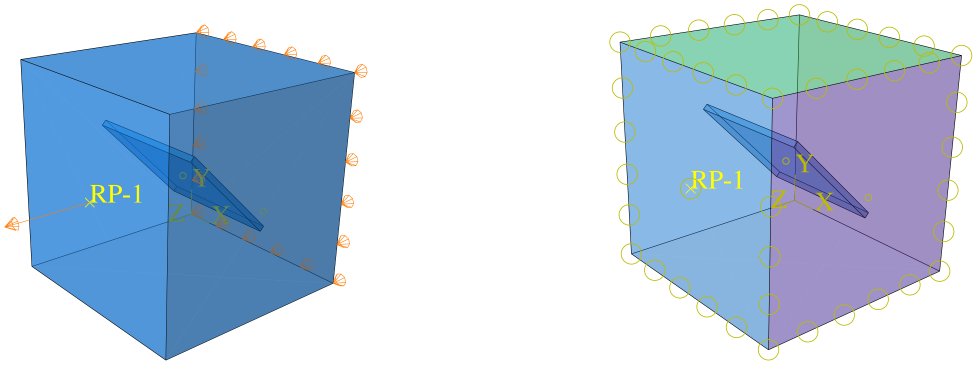
In this work, the representative volume elements (RVE) were modeled by the insertion of a carbon platelet in a metal matrix. The matrix is represented by a unit length (u.l.) cube and the platelet is a squared-base prism with 0.6 u.l. sides and with a variable thickness that is dependent on the volume fraction. In each RVE realization, the volume fraction f and the angle of orientation θ of the platelet are varied. The analyses and modeling were conducted with the Abaqus® software.

2.1 Constitutive Assuptions

For the matrix, a perfectly plastic material with Young modulus E_m = 75 GPa, Poisson's ratio ν_m = 0.3 and yield stress σ_y = 250 MPa was chosen, as to simulate a Von Mises material and avoid hardening effects. To the inclusion was assigned a elastic material with Young modulus E_g = 1 000 GPa and Poisson's ratio ν_g = 0.17.

2.2 Boundary Conditions

A uniaxial displacement condition was imposed on the face normal to the positive z axis. On the faces normal to the positive x and y axes kinematic constraints were applied (as shown in Fig. 1(a)) so that they remain plane throughout loading. A displacement of 0.01 u.l. in the reference point RP-1 was prescribed, and 0 u.l. on the opposite face (see Fig. 1(b)).

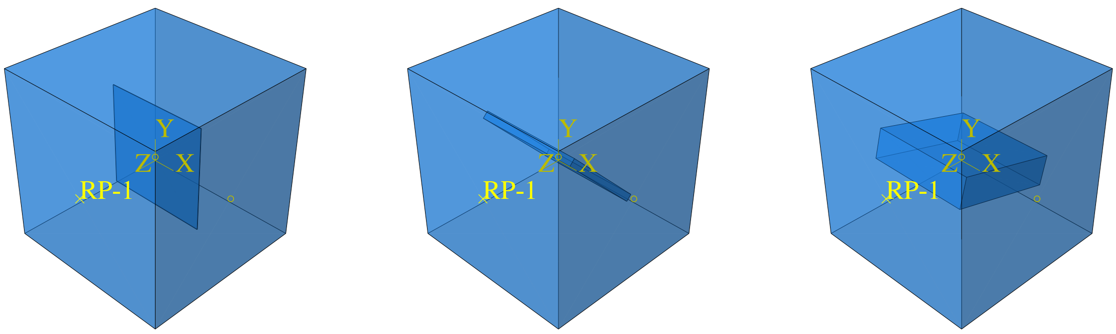


(a) (b)

Figure 1. RVE boundary conditions and constraints.

2.3 RVE Realization Parameters

The variation of the volumetric fraction of the inclusion was performed by changing its thickness, maintaining a width of 0.6 u.l. and a length of 0.6 u.l. The change in the angle of orientation was done with respect to the xy plane. Figure 2 shows a few examples of the simulated RVEs. Seven different volumetric fractions were simulated, and for each fraction, seven different angles of orientation were used, resulting in 49 models, according to Table 1.

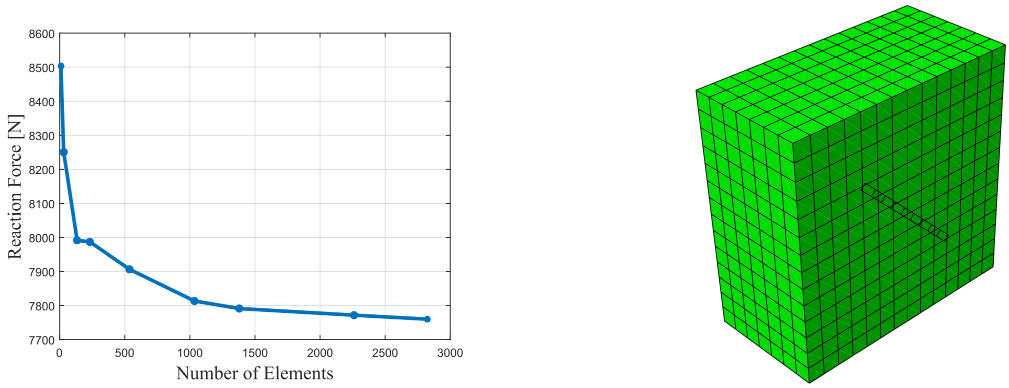


(a) (b) (c)

Figure 2. Examples of the simulated RVEs. (a) f = 0.1 %, θ = 0° ; (b) f = 1.5%, θ = 45°; (c) f = 6%, θ = 75°.

2.4 Convergence Analysis

To determine the mesh to be used on the simulations, a convergence analysis was done. The element types studied were the linear (C3D8R) and the quadratic (C3D20R) hexahedral with reduced integration. The test was done with an RVE realization with $f = 1\%$ and $\theta = 45°$ and 9 meshes were generated with the number of elements between 9 and 2825. Figure Fig. 3(a) shows the results for the values of the reaction force at the reference point for each of those meshes. In the case of the quadratic elements (not shown here), no accuracy improvements were obtained even though the computational time was greatly increased. Hence, it was decided to use a mesh of 2825 linear hexahedral elements (C3D8R), resulting in 10728 degrees of freedom. A cut of the chosen mesh is shown in Fig. 3(b).



(a) (b)

Figure 3. Convergence analysis and chosen mesh.

Additionally, two configurations of interaction techniques between the inclusion and the matrix were evaluated. One using the constraint-embedded method, and the other using the assembly-merge method. The results obtained in both cases were similar, thus, the first method was chosen, due to the easier implementation process.

3 Results

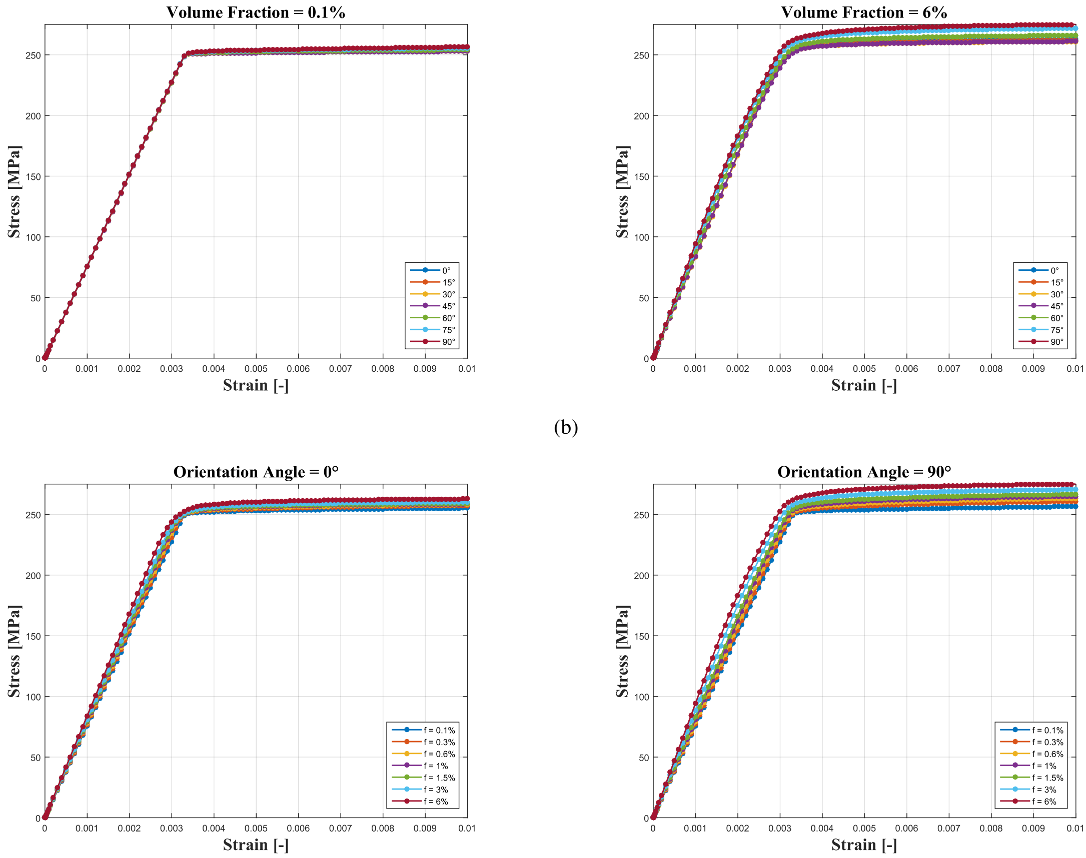
Figure 4 shows the results for a few of the simulations. The stress vs strain curves were calculated from the reaction force obtained in the simulations and using the undeformed dimensions of the RVE. With the objective of evaluating the mechanical strength of the composite, it was observed that for a deformation level of approximately 0.33%, all realizations showed signs of plastification, so the stresses associated with this deformation were stipulated as the mechanical strength for all RVE realizations. It can be noted for

It is noted that for a low volumetric fraction, the behavior of the RVE is similar to that of the matrix material, with small influence from the angle of inclination of the platelet. For a volume fraction of 6%, an increase of approximately 4% in mechanical strength is observed. 7

To better understand the influence of the angle of inclination of the platelet in the composite strength Fig. 5 was produced. It can be noted that from 0 to 45° the behavior is approximately constant. From 45° to 90° a considerable increase in resistance is observed, with the greatest strength being obtained for an inclination of 90° (with the platelet parallel to the direction of loading). Also for inclinations below 45° an increase in the volumetric fraction has a small influence on the increase in strength (250.3 MPa for $f = 1\%$ and 252.3 MPa for $f = 6\%$). On the other hand, for inclinations above 60° a greater increase in strength is observed for higher volume fractions (252.9 MPa for $f = 1\%$ and 262.1 MPa for $f = 6\%$).

4 Conclusions

This work presented a study on the influence of the volume fraction and the angle of inclination on the strength of a graphene-like material embedded in a metal matrix. Uniaxial displacement boundary conditions were imposed. To carry out the simulations, finite element models were generated using the Abaqus software. The



(a) (b) (c) (d)

Figure 4. RVE boundary conditions and constraints.

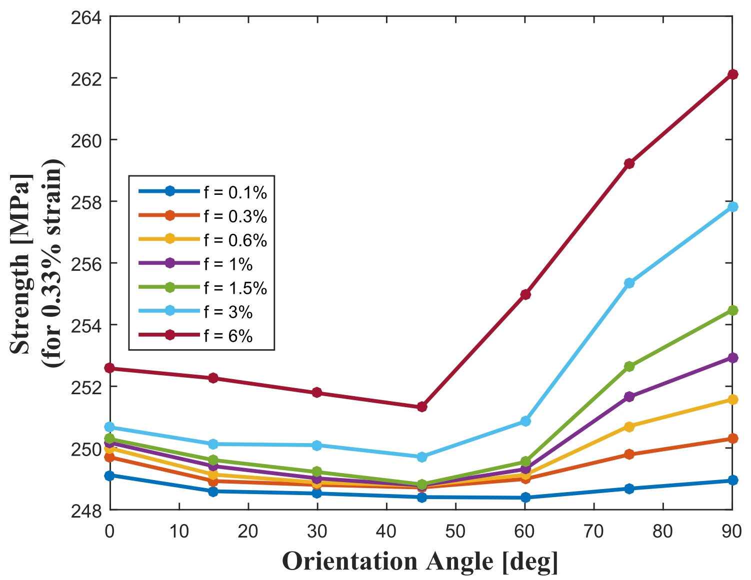


Figure 5. Mechanical strength vs angle of orientation.

results have shown that the mechanical strength is influenced by the angle of inclination of the platelet and also by its volumetric fraction, the first, having the greatest influence.

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