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Nanolaminate composites are a promising class of composites of growing interest in many engineering fields because of their high strength, light weight, and flexibility, and their ability to be tailored for specific applications [1]. It is well known that the most used construction material, cement, possesses, after hydration, a very high compressive strength but shows a low tensile strength [2]. Nano-layering of calcium-silicate-hydrate (C-S-H), the main binding phase of cement-based materials, through intercalation of graphene and graphene-derived materials can be a viable option for enhancing the tensile capacity of cement-based materials. The present work explores the mechanical properties of nanolaminate C-S-H/graphene composites and the effect of the lamella thickness (i.e., C-S-H block thickness) via molecular dynamics modeling. Tobermorite-9Å (T_9), a structural analog for C-S-H, was used as the base matrix reinforced with a single layer of embedded graphene sheets (GS) in a lamellar formation using different lamella thicknesses. The stress-strain response, elastic and shear moduli, and stiffness of the nanolaminate T_9/GS composites were investigated.

The nanostructure of the laminate T_9/GS composites were built and simulated using the open source software LAMMPS. The GS was embedded in the T_9 matrix with a lamellar orientation in the XY plane in an alternate configuration to compose representative volume elements (RVE) of the nanolaminate T_9/GS composites. The zigzag and armchair orientations of the GS were chosen along the X and Y directions, respectively. Three different RVEs were considered: (1) T_9 only, (2) T_9/GS, where 1 layer of GS was sandwiched between two blocks of T_9, and (3) T_9/3GS, where 3 layers of GS were embedded in T9 in an alternate configuration. Different lamella thicknesses were used, including 27.43Å and 7.43Å. The size of the GS was 50×50 Å. The final size of T_9 was 67×65×56.5Å with 20736 atoms, that of T_9/GS was 67×65×64 Å with 22236 atoms, and that of T_9/3GS was 67×65×54 Å with 18324 atoms. The bonded and non-bonded interactions of the different constituents of the composites were modeled using the CLAYFF forcefield for T_9 and CVFF forcefield for GS. Uniaxial tensions in the X and Y directions and shear in the XY plane were applied to obtain the stress-strain relationships of the different systems.

The density of T_9 was 2.76 g cm^{-3}, in agreement with previous studies from the literature [3]. The nanolaminate composite systems had lower density values with 2.57 g cm^{-3} and 2.46 g cm^{-3} for T_9/GS and T_9/3GS, respectively. The stress-strain curves showed that the tensile strengths of the nanolaminate composites increased in both X and Y directions with GS embedded in T_9 compared to those of T_9 alone. T_9/GS showed an increase in tensile strength of 24.6% compared to that of T_9 while 3 GS embedded in the T_9 matrix in alternate configuration increased the tensile strength of the composite by 84%. Both nanolaminate composite systems showed increase in fracture strains due to the high fracture strain of the GS itself. The percent increase in strength for the nanolaminate T_9/GS composites depended on the lamella thickness. When the lamella thickness was low (i.e., 7.43Å), the composite loading was primarily taken by the GS, resulting in higher fracture strength. The fracture point for T_9/3GS at the fracture region encompassed a post-peak region rather than a definite strain value, which indicated better flexibility of the T_9/3GS composite. Tensile strength of the nanolaminate composite in the Y direction showed the highest values for T_9/3GS among all the systems examined. For both tensile and shear strengths, the increase in fracture strains was attributed to the higher fracture strain of GS compared to T_9. The embedded GS did not affect the shear strength of T_9 as significantly as its tensile strength: the fracture shear strength of T_9/3GS and T_9/GS were 31% and 20% higher than that of T_9 alone, respectively. In contrast, the fracture shear strain of the T_9/3GS composite was considerably higher than that of the T_9/GS and T_9, significantly increasing the strain energy density.

The elastic moduli of T_9 was 110 GPa and 172 GPa in the X and Y directions, respectively. The nanolaminate T_9 composite with 3 GS showed elastic moduli of 247 GPa and 298 GPa in the X and Y directions, respectively, which represented a significant in-plane increase of 124% and 74%, respectively. The shear modulus values increased from 61.6 GPa for T_9 to 70.2 GPa for T_9/GS and 76.8 GPa for T_9/3GS (i.e., 14% and 24.5% increase, respectively). These results indicated that the nanolaminate T_9/GS composites became highly stiff along the in-plane directions where GS was in effect. Additionally, the strain energy density also increased for the nanolaminate T_9/GS composites demonstrating increased flexibility.

The primary conclusions of this study were:

- Nanolaminate T_9/GS composites with alternate GS were lightweight, with T_9/3GS having 12% lower density than T_9 itself.
- The nanolaminate architecture of T_9 with GS increased the fracture strength and fracture strain of the composite. T_9/3GS showed the highest strength and moduli compared to T_9/GS and T_9.
- The shear strain energy density of T_9/3GS was higher than that of the other systems.
- The nanolaminated architecture improves both the stiffness and flexibility of the composite.
- The strength of the laminate composite was influenced by the relative strength of the GS and T_9 matrix and was limited by the strength of the GS.

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