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Improving Interfacial Shear Strength in Graphene Reinforced Copper Nanocomposites

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Extended Abstract

Graphene has been widely used as new-generation reinforced nanofiller to achieve greatly improved mechanical properties in metal matrix nanocomposites [1, 2]. The reinforcing effect, however, has been remarkably affected by the poor interfacial interactions between graphene and metal matrix [1]. By using molecular dynamics (MD) simulations, the present work explores an effective route to improve the interfacial shear strength (ISS) of graphene sheets and graphene/Cu composites through the introduction of shear-induced wrinkles [3] and functional groups in graphene. Thereby the interfacial interaction is expected to be enhanced, leading to the improved interfacial stress transfer and eventually the mechanical properties of graphene/Cu nanocomposites. To examine the functionalization effect of graphene on the interface mechanical properties of composites, five typical functional groups, including hydrogen (-H), methyl (-CH3), ethyl (-C2H5), propyl (-C3H7), and butyl (-C4H9), are used in the present study.

The pull-out testing performed by using MD simulations indicates that the ISS between graphene sheets, as well as the graphene and the Cu matrix, increases when the graphene filler possesses shear-induced wrinkles. The maximum ISS between graphene sheets at the shear strain of 0.2 is up to 30 MPa, 84.39% higher than the case without wrinkles (16.27 MPa). While the ISS (between graphene and Cu matrix) of wrinkled graphene with the shear strain of 0.1 is 824.20 MPa, 251.48% larger than the case without wrinkles (234.49 MPa). It is also found that the functionalization of graphene can increase its surface roughness, giving rise to higher ISS. It is 249.13 MPa when the graphene is functionalized using 1% hydrogen functional groups, increased by 6.24% compared with the case without functionalization. The value further increases to 860.28 MPa after applying a shear strain of 0.1 to the hydrogen functionalized graphene. Compared with hydrogen functionalized graphene, alkyl functionalized graphene is found to be better in strengthening the interfacial interactions with the matrix. The proposed strategy of the combination of mechanical pre-shear strain and chemical surface treatment on the graphene is capable to improve the reinforcing effect of Cu nanocomposites.

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